

# **Book of Abstracts**

14th International Conference on the Physics of Non-Ideal Plasmas Rostock, September 9-14, 2012









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#### **Preface**

We welcome you to the 14th International Conference on the Physics of Non-Ideal Plasmas (PNP 14) in Rostock. The conference venue is the Steigenberger Hotel Sonne located in the heart of city. The hotel is just next to the Town Hall where the poster sessions will be held.

The 2012 conference continues a series of meetings devoted to new theoretical and experimental results on the physics of dense non-ideal plasmas: Martzlow-Garwitz 1980, Wustrow 1982, Biesenthal 1984, Greifswald 1986, Wustrow 1988, Gosen 1991, Markgrafenheide 1993, Binz 1995 (together with the 6th International Conference on the Physics on Strongly Coupled Plasmas SCP - now SCCS), Rostock 1998, Greifswald 2000, Valencia 2003, Darmstadt 2006, and Chernogolovka 2009. The PNP series was established by the Universities of Berlin, Greifswald and Rostock and by the Institute of Electron Physics of the former East German Academy of Sciences (now Paul Drude Institute in Berlin) as a platform for exchange and lively discussions on non-ideal plasmas. The close ties between German and Russian plasma physicists originate from this first period.

After 1990 the former workshop series has enlarged its spectrum to all issues concerning the physics of non-ideal plasmas. The conference is now held with a three-year period, and the topics are

- Statistical physics and ab-initio simulations,
- Producing non-ideal plasmas (optical lasers, free electron lasers, heavy-ion beams, Z machine, high explosives etc.),
- Diagnostics of non-ideal plasmas (e.g. x-ray scattering, line shapes, stopping power, emission and absorption),
- Equilibrium properties, EOS, and phase transitions,
- Kinetics, transport and optical properties,
- Dense astrophysical and ICF plasmas,
- Ultra-intense laser-matter interaction, and
- Dusty plasmas.

We would like to thank scientists from 24 countries who are attending the PNP-14 meeting in Rostock. We have received 173 papers, and the international Program Committee has assembled a very interesting program consisting of 14 invited talks, 49 topical talks, and 110 posters. This demonstrates the international character of our research and the great interest in the field of non-ideal plasmas. We would like to mention here two other series which have been established with a similar focus after 2000: the Workshops on Warm Dense Matter (WDM, since 2000) and the International Conference on High Energy Density Physics (ICHED, since 2008). Our growing community may benefit in the future from synergies between these and perhaps other meetings.

Rostock is a scenic town at the Baltic Sea founded in 1218. It is the largest town in the state Mecklenburg-Vorpommern, 220 kilometers North of Berlin and 180 kilometers East of Hamburg. The conference will be held in the Steigenberger Hotel Sonne next to the Town Hall and to the University which was founded in 1419. Many famous scientists have studied and worked here, e.g. Tycho Brahe, Joachim Jungius, Wilhelm Lenz, Otto Stern, Friedrich Hund, and Walter Schottky.

Albert Einstein received an honorary doctorate in 1919. The University of Rostock has today about 15000 students and nine faculties. An interdisciplinary faculty with four departments was founded in 2007. Physics is represented in the Department Life, Light and Matter.

Many people helped to organize the conference. I would like to thank all of them already now. We sincerely hope that all participants will enjoy the PNP-14 meeting. We are looking forward to exciting sessions and lively discussions. We also hope that you will find some time to explore our scenic town and the area. Finally, we thank the Deutsche Forschungsgemeinschaft (DFG), the SFB 652, the Wilhelm and Else Heraeus Foundation, the University of Rostock, and the Institute of Physics for support.

#### Ronald Redmer

Chairman of the Organizing Committee

### $14^{\rm th}$ International Conference on the Physics of Non-Ideal Plasmas ${\bf Conference~program}$

Monday, Sep 10		
08:45	Opening remarks	
09:00	I1 Knudson	Megaamps, Megagauss, and Megabars: Using the Sandia Z Machine to perform extreme material dynamics experiments
09:30	T2 Ternovoi	Hydrogen phase transformation under dynamic compression up to 180 GPa
09:50	T3 Dai	Transport properties of iron from warm to hot dense regime
10:10	T4 Benage	A new model for the ion-ion structure factor for warm dense matter (WDM) and implications for ion temperature mea- surements
10:30	Coffee break	
11:00	I2 Ceperley	Simulations of warm dense hydrogen
11:30	T4 Desjarlais	Entropy calculations for warm dense liquid metals
11:50	T5 Lorenzen	Nonmetal-to-metal transition in hydrogen and helium
12:10	T6 Dufty	Finite temperature quantum effects via classical methods
12:30	Coffee break	
14:00	13 Fortov	Dynamical compression of nonideal plasmas
14:30	T7 Clerouin	A database for pressure and electrical resistivity measurements on hot expanded metals
14:50	T8 Recoules	Ab initio calculation of X-ray absorption spectra for warm dense matter
15:10	T9 Ziaja-Motyka	Simulations of FEL-excited matter
15:30	Coffee break	
16:00	14 Koenig	Direct laser-driven quasi-isentropic compression of iron relevant for Earth-like planets interiors
16:30	T10 Mazevet	Ab initio calculations of the properties of SiO <sub>2</sub>
16:50	T11 Gamaly	Warm dense matter produced by fs-laser- triggered confined micro-explosion
17:10	T12 Matsuda	Compton scattering study of expanded fluid alkali metals
17:30	HEDgeHOB Coll	aboration Board Meeting
19:00 20:00	Guided tour through the University of Music and Drama (HMT) Concert: University of Music and Drama (HMT)	

Tuesday, Sep 11			
09:00	I5 Glenzer	Update on experiments on the National Ignition Facility	
09:30	T13 Fletcher	X-ray Thomson scattering measurements of temperature	
		and density from multi-shocked CH capsules	
09:50	T14 Hamel	First-principles molecular dynamics simulations of the equa-	
		tion of state of plastic ablators for ICF	
10:10	T15 Mintsev	Proton radiography of nonideal plasma	
10:30	Coffee break		
11:00	l6 Fortney	Examining the interior structure of transiting extrasolar gi-	
		ant planets	
11:30	T16 Nettelmann	Jupiter as an ideal planet to study non-ideal plasmas	
11:50	T17 Potekhin	Thermonuclear fusion in dense stars: Electron screening and	
		conductive cooling effects	
	T18 Gryaznov	SAHA-S – thermodynamic model of solar plasma	
12:30	Coffee break		
14:00	17 Falcone	X-ray studies of warm and dense matter	
14:30	T19 Döppner	Ultrafast transitions from solid graphite to plasma states	
		induced by x-ray free-electron laser puls	
14:50	T20	Probing dense plasmas by x-ray scattering and spectroscopy	
	Tschentscher	at European XFEL	
15:10	T21 Rosmej	Properties of hydrodynamic stable non-ideal plasma ob-	
		tained via X-ray heating of low density foams	
15:30	Coffee break		
16:00	18 Gericke	Effective interactions and ion dynamics in warm dense mat-	
		ter	
	T22 Sperling	Thomson scattering on inhomogeneous targets	
16:50	T23 Rozmus	Linear plasma response, electrostatic fluctuations and	
45.40	T0 ( E) 1 1	Thomson scattering	
17:10	T24 Tkachenko	The extended Mermin approximation for the collisional	
17.90	D + C : I	plasma dielectric function	
17:30	Poster Session I (Town Hall)		
19:30	Tour 1: Astronomical Clock Marienkirche Tour 2: Nightwells through Old Town		
20:30	Tour 2: Nightwalk through Old Town		

Wednesday, Sep 12		
09:00	19 Keitel	Extremely high-intensity laser interactions with fundamen-
		tal quantum systems
09:30	T25 Liseykina	Ionization dynamics in laser-irradiated droplets
09:50	T26 Andreev	A wide-range model of intense laser interaction with matter
10:10	T27 Kull	Quantum plasma simulations beyond the semiclassical ap-
		proximation
10:30	Coffee break	
11:00	I10 Goree	Physics of liquid-phase dusty plasmas
11:30	T28 Petrov	Ordering and transport phenomena in strongly coupled sys-
		tems of charged dust in traps and plasmas
11:50	T29 Starostin	Dust acoustic waves in non-equilibrium plasmas at elevated
		pressure
12:10	T30 Kopnin	Anomalously high dust particle charging by an electron
		beam
13:00	Excursion to Stralsund ("Ozeaneum" and "Old Town")	

	Thursday, Sep 13		
09:00	I11 Killian	Beyond Landau-Spitzer: Collision rates in strongly coupled	
		ultracold plasmas	
09:30	T31 Ott	Nonideal plasmas in a strong magnetic field	
09:50	T32 Kalman	Acoustic and optic modes in strongly coupled binary liquids	
		and solids	
10:10	T33 Mulser	Dynamic shielding, antishielding, cut offs, and the Coulomb	
		paradox	
10:30	Coffee break		
11:00	I12 Zhang	Transport properties and equation of states for dense	
		deuterium-tritium plasmas	
11:30	T34 Trickey	Constraint-based development of orbital-free free energy	
		density functionals	
11:50	T35 Morozov	Simulation of electron propagation in nonideal plasmas us-	
		ing split wave packet molecular dynamics	
12:10	T36 Ramazanov	Dynamical properties of nonideal plasma on the basis of	
		effective potentials	
12:30	Coffee break		
14:00	<b>I13</b> Ng	Electron energy transport and AC conductivity of nonequi-	
		librium warm dense gold	
14:30	T37 Ludwig	Multiscale Approach to Strongly Correlated Multi-	
	= C 111	component Plasmas in Nonequilibrium	
14:50	T38 Collins	Mass transport in warm, dense matter conditions	
15:10	T39 Norman	Recombination in dense ion plasmas	
15:30			
16:00		Laser shock experiments for materials of giant planets	
16:30	T40 Yoneda	Ultra-short transient state of metals produced by intense	
		femtosecond EUV laser	
16:50	T41 Krainov	Ionization of atoms by intense attosecond pulses	
17:30	Poster Session II		
19:30	Conference Dinner: "Lokschuppen" (City Harbour)		

Friday, Sep 14			
09:00	T42 Tahir	Ion beam driven high energy density physics studies at FAIR	
		at Darmstadt	
09:20	T43 Deutsch	He-like effective interactions for WDM plasmas	
09:40	T44 Hazak	A Resolved-Super-Transition-Arrays method for calculation	
		of the spectral absorption coefficient in hot plasmas	
10:00	T45 Schram	Anomalous diffusion on the basis of the extended master	
		equation	
10:20	Coffee break		
10:50	T46 Fennel	Fully microscopic analysis of laser-driven plasmas via mi-	
		croscopic particle-in-cell simulations (MicPIC)	
11:10	T47 Winkel	Electronic correlations in nanoclusters - Molecular dynamics	
		simulations	
11:30	T48 Moll	Inverse bremsstrahlung heating in noble gas clusters irradi-	
		ated by femtosecond laser pulses	
11:50	T49 Raitza	Response of excited nano plasmas due to collective electron	
		dynamics	
12:10	Closing remarks		
14:00	Departure		



Abstracts of talks Monday 10.09.2012, 9:00 - 17:30 **I1**: Monday 10.09.2012, 9:00 - 9:30

### Megaamps, Megagauss, and Megabars: Using the Sandia Z Machine to perform extreme material dynamics experiments

Marcus D. Knudson<sup>1</sup>

For the past decade, a large, interdisciplinary team at Sandia National Laboratories has been refining the Z Machine (20+ MA and 10+ MGauss) into a mature, robust, and precise platform for material dynamics experiments in the multi-Mbar pressure regime. In particular, significant effort has gone into effectively coupling condensed matter theory, magneto-hydrodynamic simulation, and electromagnetic modeling to produce a fully self-consistent simulation capability able to very accurately predict the performance of the Z machine and various experimental load configurations. This capability has been instrumental in the ability to develop experimental platforms to routinely perform magnetic ramp compression experiments to over 4 Mbar, and magnetically accelerate flyer plates to over 40 km/s, creating over 20 Mbar impact pressures. Furthermore, a strong tie has been developed between the condensed matter theory and the experimental program. This coupling has been proven time and again to be extremely fruitful, with the capability of both theory and experiment being challenged and advanced through this close interrelationship. This presentation will provide an overview of the material dynamics platform and discuss several examples of the use of Z to perform extreme material dynamics studies with unprecedented accuracy in support of basic science, planetary astrophysics, inertial confinement fusion, and the emerging field of high energy density laboratory physics.

<sup>&</sup>lt;sup>1</sup>Sandia National Laboratories, Albuquerque NM 87123 \*

<sup>\*</sup> Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

T1: Monday 10.09.2012, 9:30 - 9:50

### Hydrogen phase transformation under dynamic compression up to 180 GPa

Ternovoi V.Ya.<sup>1</sup>

Thermodynamic and transport properties of hot compressed hydrogen are important for research of fusion and giant planet interiors [1]. Now, a phase diagram of hydrogen is not well defined. The most difficult for description is pressures lower 500 - 800 GPa and temperatures of 1000 - 10000 K. Understanding of mechanism of hydrogen transformation into a state with high electrical conductivity is of great theoretical interest [1].

In this work, results of measurements of electrical conductivity of layers of initially gaseous hydrogen multiple shock-compressed up to the pressure 120 – 180 GPa and temperature 4000 – 10000 K are presented. Decrease of the conductivity from 424 to 20 S/cm with temperature increasing from 2700 to 6000 K along the 135 GPa isobar was registered. Along the 180 GPa isobar the specific conductivity is decreased from 1100 S/cm (at T = 6400 K) up to 100 S/cm (at T = 6900 K). These states locate near the boundary of dielectric – metal transformation region, according to multi-phase EOS [2]. Also, the results of measurements of optical emission intensity of hydrogen during dynamic compression up to 100 - 150 GPa are presented. Initial density of gaseous hydrogen sample cooled by liquid nitrogen was defined by its initial pressure at 77 K. Brightness temperatures obtained for maximum pressure states are within 2500 – 7000 K. A temperature peak near the end of compression was observed in all experiments. The shape of measured temperature profiles vs time qualitatively differs from the shapes obtained from hydrodynamic simulation based on multiphase hydrogen equation of state [2]. This fact is explained by forming the hydrogen metallic phase film on the cold surface of LiF window. In experiments with T=6800K at maximum compression and pressure about 150 GPa, the temperature shape corresponds to the properties of dielectric phase of hydrogen according to model [2]. In these experiments the optical transparency of hydrogen layer was detected. In the pressure – temperature diagram the maximum compression states with dielectric and metallic behavior are according to the phase boundaries predicted by EOS model [2].

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<sup>[1]</sup> Fortov, V. E., Khrapac, A. G., Yakubov, I. T., "Physics of Strongly Coupled Plasmas", Oxford University Press, 2005.

<sup>[2]</sup> A.A.Pyalling. Semiempirical multiphase equation of state for hydrogen. High Temperature, Vol. 48, No.2, pp.163 - 169

**T2**: Monday 10.09.2012, 9:50 - 10:10

#### Transport properties of iron from warm to hot dense regime

#### Jiayu Dai<sup>1</sup>

The transport properties, including diffusion, viscosity, thermal and electrical conductivities are calculated from the first principles molecular dynamics called quantum Langevin molecular dynamics [1,2]. The two initial phases are considered, which are BCC and FCC structures with two densities of 33.385 g/cm<sup>3</sup> and 45 g/cm<sup>3</sup> and the temperatures in 1-10 eV. In particular, the transport properties along the Hugoniot curve up to 100 eV [3] are discussed, showing the significant effect of ordered structures [4].

- [1] J. Dai, Y. Hou, and J. Yuan, Phys. Rev. Lett. 104, 245001 (2010).
- [2] J. Dai, Y. Hou, and J. Yuan, APJ, 721, 1158 (2010).
- [3] J. Dai, D. Kang and Z. Zhao et al. arXiv:1109.4252v2 .
- [4] J. Dai, Y. Hou, and J. Yuan, High Energy Density Physics, 7: 84-90 (2011).

<sup>&</sup>lt;sup>1</sup>Department of Physics, National University of Defense Technology, Changsha, 410073, China

**T3**: Monday 10.09.2012, 10:10 - 10:30

#### A new model for the ion-ion structure factor for warm dense matter (WDM) and implications for ion temperature measurements

John F Benage<sup>1</sup>, Michael S Murillo<sup>1</sup>, Liam Stanton<sup>2</sup>, Michael P Desjarlais<sup>3</sup>

X-ray Thomson scattering measurements are becoming increasingly common in dense plasma and WDM experiments. These measurements are proving to be a very powerful diagnostic tool to characterize the material conditions in the experiments and enabling the determination of many properties of dense plasmas and WDM. In many of these experiments, the electron and ion temperatures may not be in equilibrium, due to the manner of creating the WDM conditions. Measurements of the ion temperature in such experiments would be extremely valuable for characterizing the material conditions. It has been proposed that using x-ray Thomson scattering data, one can determine the ion temperature, provided the ion-ion structure factor is known. To investigate this novel idea, we have developed a new model using linear response coupled with the finite temperature Lindhard susceptibility and HNC calculations to determine the ion-ion structure factor in WDM. We compare our model to data where available, to other models, and to QMD simulations. We find this new model compares very well to the QMD at temperatures above 1 eV for a variety of materials. However, so little data exists in the WDM region that none of the models have been validated at those conditions. In addition, because these models can predict very different answers at small wavenumbers, the implications for ion temperature measurements are severe. Some ideas for resolving these issues to enable ion temperature measurements for WDM will be presented.

<sup>&</sup>lt;sup>1</sup>Los Alamos National Laboratory

<sup>&</sup>lt;sup>2</sup>Lawrence Livermore National Laboratory

<sup>&</sup>lt;sup>3</sup>Sandia National Laboratories

**12**: Monday 10.09.2012, 11:00 - 11:30

#### Simulations of warm dense hydrogen

David Ceperley <sup>1</sup>

Recent advances in computer hardware and simulations methods have allowed us to perform much more accurate simulations of dense hydrogen using both "First principles Molecular Dynamics" (based on DFT) and "Coupled Electron-Ion Monte Carlo" (based on Quantum Monte Carlo). We will discuss results for the liquid-liquid phase transition in dense hydrogen and for the principal Hugoniot. We find [1] that that the density functional and the quantum motion of the protons have a major effect on the liquid-liquid transition.

Supported by DOE DE FG52-09-NA29456 and INCITE award MAT038. [1] M. A. Morales, J. M. McMahon, C. Pierleoni, and D. M. Ceperley "Nuclear Quantum Effects and Non-Local Exchange-Correlation Functionals in Liquid Hydrogen at High Pressure", submitted Physical Review (2012).

<sup>&</sup>lt;sup>1</sup>Department of Physics, University of Illinois at Urbana-Champaign

**T4**: Monday 10.09.2012, 11:30 - 11:50

#### Entropy calculations for warm dense liquid metals

Michael Desjarlais<sup>1</sup>

The total entropy is not an easily accessible explicit quantity in first principles molecular dynamics simulations. However, it is an extremely important quantity for the calculation of total free energies and derived quantities such as phase boundaries. In this talk I will discuss recent advances in the direct calculation of the entropy of warm dense liquid metals using quantum molecular dynamics simulations with density functional theory. I will compare the results to data and the results of indirect methods, such as the two-phase simulation method to determine phase boundaries.

<sup>&</sup>lt;sup>1</sup>Sandia National Laboratories, Albuquerque, New Mexico, USA\*

<sup>\*</sup> Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**T5**: Monday 10.09.2012, 11:50 - 12:10

#### Nonmetal-to-metal transition in hydrogen and helium

Winfried Lorenzen<sup>1</sup>, Bastian Holst<sup>2</sup>, Andreas Becker<sup>1</sup>, Ronald Redmer<sup>1</sup>

Hydrogen-helium mixtures have long been predicted to undergo demixing at high pressures of several megabar which occur in the interiors of giant planets such as Jupiter and Saturn. This effect is most important to understand their evolution and current interior structure. Ab initio calculations have already proven their potential to give precise predictions for the properties of matter under these extreme conditions. Here we present results for the miscibility gap at high pressures obtained from ab initio molecular dynamics simulations [1]. By using the Kubo-Greenwood formula we calculate the electrical conductivity and reveal the close connection between the location of the miscibility gap and the nonmetal-to-metal transition [2]. We also discuss the first-order nature of this transition in hydrogen [3] and its potential occurence in hydrogen-helium mixtures.

- [1] Lorenzen W., Holst B., Redmer R., Phys. Rev. Lett. 102, 115701 (2009).
- [2] Lorenzen W., Holst B., Redmer R., Phys. Rev. B 84, 235109 (2011).
- [3] Lorenzen W., Holst B., Redmer R., Phys. Rev. B 82, 195107 (2010).

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<sup>&</sup>lt;sup>2</sup>CEA, DAM, DIF, F-91297 Arpajon, France

**T6**: Monday 10.09.2012, 12:10 - 12:30

#### Finite temperature quantum effects via classical methods

Sandipan Dutta<sup>1</sup>, <u>James Dufty</u><sup>1</sup>

<sup>1</sup> University of Florida

A quantum system at equilibrium is represented by a corresponding classical system, chosen to reproduce thermodynamic and structural properties. The motivation is to allow application of classical strong coupling theories and simulation to quantum systems at strong coupling. The correspondence is made at the level of the grand canonical ensembles for the two systems. An effective temperature, local chemical potential, and pair potential are introduced to define the corresponding classical system. These are determined formally by requiring the equivalence of the grand potentials and their functional derivatives. Practical inversions of these formal definitions are indicated via the integral equations for pair correlation functions of classical liquid theory. Two illustrations of applications are discussed: the thermodynamics and structure of uniform jellium over a range of temperatures and densities, and the shell structure of harmonically bound charges.

Research supported in part by US DoE Grant DE-SC0002139.

**I3**: Monday 10.09.2012, 14:00 - 14:30

#### Dynamical compression of nonideal plasmas

V.E. Fortov<sup>1</sup>

The physical properties of strongly coupled plasmas at extremely high energy densities are analyzed in a broad region of the phase diagram. The theoretical and experimental methods of hot dense plasma investigations are discussed. Main attention is paid to shock wave methods. Intense shock, rarefaction waves in gaseous, solid and porous samples were generated by high hypervelocity impacts, explosions, bulk electrons and relativistic ions and lasers. The highly time-resolved diagnostics allow us to measure the thermodynamic, radiative and mechanical properties of high temperature plasma in a broad region of the phase diagram from compressed condensed solid states up to the low density gas range, including high temperature evaporation curves with near-critical states of metals, strongly coupled plasma, and metal-insulator transition regions.

Thermodynamic parameters of metal critical points are analyzed and compared with the theoretical predictions. The theoretical interpretation of the opacity measurements demonstrates strong deformation of discrete spectrum in coupled materials. "Pressure ionization" phenomena in hydrogen, iodine, silica, sulfur, fullerenes, and some metals are analyzed on the base of multiple shock compression experiments. Analytical models based on the shift of ionization equilibrium are presented. The quantum Monte Carlo calculations and density functional theory were used for theoretical interpretation of the "pressure ionization" of plasma. The effect of "dielectrization" for some metals (Li, Na) are discussed on the base of multiple shock compression experiments. The theoretical models and experiments on plasma phase transition in nonideal plasma are discussed.

Strongly coupled multicomponent plasma thermodynamical models were applied for theoretical description of the Sun interior.

<sup>&</sup>lt;sup>1</sup>Joint Institute for High Temperature of RAS, Moscow 125412 Russia

**T7**: Monday 10.09.2012, 14:30 - 14:50

#### A database for pressure and electrical resistivity measurements on hot expanded metals

J. Clérouin<sup>1</sup>

We discuss experimental results on equation of state and resistivities of various expanded metals. Data are presented for aluminum (0.1 and 0.3 g/cm<sup>3</sup>), nickel (0.2  $g/cm^3$ ), titanium(0.1  $g/cm^3$ ), copper (0.3 and 0.5  $g/cm^3$ ), silver (0.43  $g/cm^3$ ), gold (0.5 g/cm<sup>3</sup>), boron(0.094 g/cm<sup>3</sup>) and silicon (0.21 g/cm<sup>3</sup>) for temperatures ranging from 0.5 eV to 3-4 eV. Such thermodynamic conditions corresponds to the warm dense matter (WDM) regime. These data are used to benchmark different theoretical approaches [1,2]. A comparison with fully 3-dimensional quantum molecular dynamics (QMD) simulations, based on density functional theory, allows for the evaluation of the experimental temperature, that is not accessible to the measurements, and allows for building useful data tables gathering energy, pressure, conductivity and temperatures. Average atom (AA) methods, that are essentially one dimensional, are also tested for a fast evaluation of plasma properties. Ionization, deduced from AA calculations, is used as input parameter for plasma formulations. If we get a general good agreement between the different approaches, we still observe descrepancies between theories for some well identified regimes (dimers formation at low density, resonance states at high density) making such experimental data particularly precious in the WDM regime.

- [1] J. Clérouin, C. Starrett et al., Contrib. Plasma Phys., 52(1),17-22, (2012).
- [2] J. Clérouin, P. Noiret et al., submitted to Physics of Plasmas (2012).

<sup>&</sup>lt;sup>1</sup>CEA, DAM, DIF, 91297 Arpajon, France

**T8**: Monday 10.09.2012, 14:50 - 15:10

### Ab initio calculation of X-ray absorption spectra for warm dense matter

<u>Vanina Recoules</u><sup>1</sup>, Stephane Mazevet<sup>2</sup>
<sup>1</sup> CEA-DAM-DIF
<sup>2</sup> LUTH - Observatoire de Paris

The prospect of extending the characterization of dense plasmas and shock compressed matter to near edge absorption spectroscopy is very appealing both from a theoretical and an experimental side. Measurements of near edge absorption spectra of shock compressed matter brings invaluable information on the evolution of the electronic structure as the system is subject to a significant increase in both pressure and temperature. This measurements severally constrains theoretical approaches currently used. From the theoretical side, the use of ab initio electronic structure approaches based on density functional theory (DFT) combined with molecular dynamics simulations and linear response theory has been rather successful at providing, to first order, a satisfying description of this complex state of matter. However, the transport properties calculated have been so far limited to low frequencies (below 100eV). In this context, we have developed a first principle approach to calculate the near edge absorption spectrum (XANES) of dense plasmas based on density functional electronic structure calculations and molecular dynamics simulations. This approach provides a first principle description of both the electronic structure and the thermodynamics state of the system. The calculation of the K-edge shift when increasing density and/or temperature formally requires a fully self-consistent calculations beyond the frozen core approximation. A special care is needed to design the Projected Augmented Wave database to be able to describe excited states of high energy. This method was first applied for the calculation of the XANES spectra of warm dense aluminum and was compared to experimental results. We have then applied this method to the calculation of the XANES spectra and K-edge shift of iron at solid density for temperature around the melting temperature. Calculations for iron are far more complex than those for aluminium. We show how XANES spectra can be used to diagnose solid-solid and solid-liquid phase transition.

**T9**: Monday 10.09.2012, 15:10 - 15:30

#### Simulations of FEL-excited matter

 $\frac{\text{Beata Ziaja-Motyka}^1}{^1CFEL, DESY, Hamburg}$ , Nikita Medvedev<sup>1</sup>

We apply continuum approach to follow the dynamics of irradiated complex samples. First we discuss its advantages and limitations when compared to other modelling methods. We then apply this approach to describe data on irradiated clusters and laser-created plasmas that were recorded at the free-electron-laser FLASH facility at DESY Hamburg. We show a good agreement between experimental results and our theoretical estimations. Finally we give an outlook on applying the continuum approach (combined with tight binding molecular dynamics technique) to describe ultrafast transitions within FEL-excited solids.

**I4**: Monday 10.09.2012, 16:00 - 16:30

### Direct laser-driven quasi-isentropic compression of iron relevant for Earth-like planets interiors

M. Koenig<sup>1</sup>, N. Amadou<sup>1</sup>, E. Brambrink<sup>1</sup>, T. Vinci, A. Benuzzi-Mounaix<sup>1</sup>, F. Guyot<sup>2</sup>, G. Morard<sup>2</sup>, G. Huser<sup>3</sup>, K. Myanishi<sup>4</sup>, N. Ozaki<sup>4</sup>, R. Kodama<sup>4</sup>, T. de Rességuier<sup>5</sup>, S. Mazevet<sup>6</sup>, O. Henry<sup>7</sup>, D. Raffestin<sup>7</sup>

Quasi-isentropic laser driven compression on materials relevant to Earth-like planet interiors allow to access thermodynamical parameters directly connected to the extreme conditions (330-1500 GPa, 5000-8000 K) of those objects. Here, I will present two series of experiments performed recently on LULI2000 and LIL facility. In both experiments a laser ramp profile system was used in order to compress the target as isentropic as possible. At LULI, with laser energy (300 J, 2  $\omega$ , 4 ns) pressures up to 100 GPa were obtained. Different pressure ramp shapes, corresponding to different loading rates, were used to investigate the alpha-epsilon transition dynamics. On the LIL facility, a much higher energy and longer ramp (2.5 kJ, 3  $\omega$ , 20 ns) allowed to compressed iron up to 900 GPa. In the meanwhile, temperature given by a rear side Streaked Optical pyrometer showed a value almost similar to the one expected in telluric planetary cores. All results will be presented, compared to simulations and discussed.

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**T10**: Monday 10.09.2012, 16:30 - 16:50

#### Ab initio calculations of the properties of SiO<sub>2</sub>

 $\underline{S.~Mazevet}^1,~T.~Tsushiya^1,~F.~Guyot^1,~A.~Denoeud^1,~A.~Benuzzi^1,~A.~Ravasio^1$   $^1LUTH~Observatoire~de~Paris$ 

Using ab initio simulations, we investigate the properties of SiO<sub>2</sub> at conditions encountered in planetary cores. We determine the high pressure melting curve of silica up to conditions corresponding to Saturn inner core using the two phases approach. Using the Kubo-Greenwood formulation, we also calculate the transport properties. We find that metallization is closely related to the variation of the coordination number Si-O and identify detectable signature in the XANE spectra.

**T11**: Monday 10.09.2012, 16:50 - 17:10

### Warm dense matter produced by fs-laser- triggered confined micro-explosion

E.G. Gamaly <sup>1</sup>, A. Vailionis<sup>2</sup>, V. Mizeikis<sup>3</sup>, W. Yang<sup>4</sup>, A.V. Rode<sup>1</sup>, S. Juodkazis<sup>5</sup>

We report the experimental evidence for producing WDM at laboratory tabletop by fs-laser tightly focused inside a transparent crystal. The solid density non-ideal plasma at absorbed energy density of MJ/cm<sup>3</sup> maintains temperature several tens of eV, pressure of TPa during a picosecond time followed by explosion confined inside a crystal. Synchrotron X-ray diffraction analysis revealed the presence in laser-affected sapphire of new super-dense bcc-Al, never observed before. In non-equilibrium conditions dominated by the Coulomb interactions shock wave front has a complicated structure with light and heavy ions separated in space. Analysis shows that the ions space separation and fast cooling resulted in formation of new crystal. We qualitatively follow the changes in material properties from room temperature to the dense and hot star-core-like plasma of WDM. The brief account of recent experiments with crystals of diamond and olivine will be presented. We show that fs-laser induced micro-explosion confined inside a transparent solid opens new routes for synthesis of new materials and study of WDM at a laboratory bench-top.

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T12: Monday 10.09.2012, 17:10 - 17:30

#### Compton scattering study of expanded fluid alkali metals

<u>K. Matsuda</u><sup>1</sup>, T. Fukumaru<sup>1</sup>, K. Kimura<sup>1</sup>, Y. Kajihara<sup>2</sup>, M. Inui<sup>2</sup>, K. Tamura<sup>3</sup>, M. Yao<sup>1</sup>, M. Itoh<sup>4</sup>, Y. Sakurai<sup>4</sup>

Liquid alkali metals near the melting point behave as a simple monatomic metal-lic liquid, whereas alkali metal vapors are an insulator which consists of monomers, dimers in equilibrium. These facts tell us that fluid alkali metals finally experience a metal-insulator (M-I) transition with volume expansion. The M-I transitions of fluid alkali metals occur around the critical density [1]. The interrelation between the liquid-vapor phase transition and the M-I transition has been a fundamental issue in condensed matter physics and its elucidation requires microscopic observation for how atoms and molecules are formed from a condensed metallic liquid (strongly coupled electron-ion plasma).

We have thus far performed x-ray diffraction and small angle x-ray scattering measurements for fluid rubidium and cesium up to supercritical regions using synchrotron radiation at SPring-8. The experimental results show that the nearest neighbor distance starts to decrease and the density fluctuation increases below the density of 1.1 g/cc for rubidium and 1.3 g/cc for cesium, respectively. These structural features indicate the emergence of spatial atomic-density fluctuations in the fluid. We speculate that the attractive force among ions is enhanced with decreasing density and the charge fluctuations of the low-density interacting electron gas play an essential role for that enhanced attractive force [2].

X-ray Compton scattering using synchrotron radiation has been a well-established technique for measuring the electron momentum density in materials and also provides a valuable opportunity to perform the experiments on the electronic state under the extreme conditions such as high temperatures and pressures. We have developed a high pressure vessel and a sample cell specially designed for x-ray Compton scattering experiments of fluid alkali metals and succeeded to measure Compton profiles of fluid rubidium from near the melting point up to supercritical regions ( 2100 K and 13.0 MPa). It was found that the difference between the experimentally obtained Compton profiles and those estimated by the free electron gas (FEG) model was pronounced with volume expansion, indicating that the electronic states deviate from those of the FEG with decreasing fluid density.

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<sup>&</sup>lt;sup>4</sup>SPring-8/JASRI

<sup>[1]</sup> F. Hensel and W.W. Warren, Jr., Fluid Metals; Liquid-Vapor Transition of Metals, (Princeton, NJ, 1999).

<sup>[2]</sup> K. Matsuda, K. Tamura, M. Inui, Phys. Rev. Lett., 98, 096401 (2007).



Abstracts of talks Tuesday 11.09.2012, 9:00 - 17:30

**I5**: Tuesday 11.09.2012, 9:00 - 9:30

#### Update on experiments on the National Ignition Facility\*

S.H. Glenzer<sup>1</sup>

With completion of the National Ignition Facility (NIF) at the Lawrence Livermore National Laboratory the quest for producing a burning fusion plasma has begun. The goal of these experiments is to compress matter to densities and temperatures higher than the interior of the sun to initiate nuclear fusion and burn of hydrogen isotopes [1]. The first inertial confinement fusion implosion experiments with cryogenic fuel layers have recently been fielded. These experiments use mega joule laser energies that compress fusion capsules in indirect drive hohlraums to test initial hot spot formation and thermonuclear fuel assembly. We applied 0.17 mg of equimolar deuterium-tritium thermonuclear fuel with the potential for ignition and significant fusion yield conditions. Measurements of the implosion core, neutron yield, temperatures and fuel areal density show compression by a factor of 30 to a fuel density of over 500 g/cc and hot spot temperature of 3.5 keV resulting in a stagnation pressures of more than 100 Gbar. This achievement is the result of the first hohlraum and capsule tuning experiments where the stagnation pressures have been systematically increased by more than a factor of 10 by fielding low-entropy implosions through the control of radiation symmetry, small hot electron production, and proper shock timing. These implosions demonstrate high Lawson-type fusion confinement parameters of 10 atm s where the comparison with radiation-hydrodynamic simulations indicates that these implosions are within a factor of three required for reaching ignition and high yield. In this talk we will discuss recent findings indicating the path towards further pressure increases for the near future.

\*This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

[1] S.H. Glenzer, B.K. Spears, M.J. Edwards et al., "First implosion experiments with cryogenic thermonuclear fuel on the National Ignition Facility", Plasma Physics and Controlled Fusion 54, 045013 (2012).



Picture of a cryogenic ignition target before enclosed by the shroud. The hohlraum contains a spherical 2.2-mm diameter capsule and the thermonuclear fuel layer.

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T13: Tuesday 11.09.2012, 9:30 - 9:50

# X-ray Thomson scattering measurements of temperature and density from multi-shocked CH capsules

<u>L. Fletcher</u><sup>1,2,3</sup>, A. Kritcher<sup>3</sup>, A. Pak<sup>3</sup>, T. Ma<sup>3</sup>, T. Döppner<sup>3</sup>, C. Fortmann<sup>3,4</sup>, R.W. Lee<sup>3</sup>, J.J. Lee<sup>3</sup>, O.L. Landen<sup>3</sup>, S.H. Glenzer<sup>3</sup>, R.W. Falcone<sup>1,2</sup>

To achieve the high level of compression, at low entropy, needed for inertial confinement fusion (ICF) currently requires the use of multiple coalescing shock waves. We report on direct measurements of the electron densities, electron temperatures, and ionization states of spherically compressed three-shocked CH capsules through the use of spectrally resolved X-ray Thomson scattering. A total of 45 beams (13.5 kJ incident on a CH shell) from the OMEGA laser system at 300 J/beam are used to compress a 70 micron thick CH shell above solid-mass density using three coalescing shocks. Separately, a laser-produced high energy Zinc He- $\alpha$  X-ray source at 9 keV delayed approximately 200 ps - 800 ps in time after maximum compression is used to probe the plasma under a non-collective scattering geometry. This scattering geometry is simultaneously measured at both large and small scattering angles of 135 and 75 degrees respectively. These measurements can provide a full characterization of the heating process, enabling a complete description of the time-dependent hydrodynamic evolution of shock-compressed CH capsules and can be used as a platform to study current equation of state models of CH under such extreme conditions.

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**T14**: Tuesday 11.09.2012, 9:50 - 10:10

# First-principles molecular dynamics simulations of the equation of state of plastic ablators for ICF

<u>Sebastien Hamel</u><sup>1</sup>, Lorin X. Benedict<sup>1</sup>, Phillip A. Sterne<sup>1</sup>, Eric Schwegler<sup>1</sup> <sup>1</sup>Lawrence Livermore National Laboratory

We report the computation of the equation of state of a plastic with stoichiometry CH1.36, which is similar to a material currently being used as an ablator in inertial confinement fusion capsules. The computational scheme employed is density functional theory-based molecular dynamics, and the conditions considered are:  $1.8~\rm g/cm^3 < \rho < 10~\rm g/cm^3$ , and  $4{,}000~\rm K < T < 100{,}000~\rm K$ . After fitting the computed pressure and internal energy with a Mie-Grüneisen free energy model, we predict the principal shock Hugoniot and various shock-and-release paths and show that they agree with recent experimental data. We also establish that, at least in the particular  $(\rho, T)$ -range considered, the equation of state of this material is well-described by an equal pressure and temperature mixture of pure C and H equations of state with a stoichiometry-weighted additive-volume assumption.

**T15**: Tuesday 11.09.2012, 10:10 - 10:30

#### Proton radiography of nonideal plasma

Mintsev V.B.<sup>1</sup>, Kolesnikov S.A.<sup>1</sup>, Dudin S.V.<sup>1</sup>, Lavrov V.V.<sup>1</sup>, Utkin A.V.<sup>1</sup>, Shilkin N.S.<sup>1</sup>,

Fortov V.E.<sup>1</sup>, Turtikov V.I.<sup>2</sup>, Golubev A.A.<sup>2</sup>, Sharkov B.Yu.<sup>2</sup>, Kantsirev A.A.<sup>2</sup>

In recent years studies of shock and detonation wave phenomena at extreme conditions have been conducted at proton radiography facility developed at the ITEP Terawatt Accelerator (TWAC-ITEP). The 800 MeV proton beam intensity in these experiments is about 1010 particles per pulse. A single beam bunch consists of four consequent 70 ns long micro bunches with 250 ns intervals between them. The spatial resolution of the facility that was measured in static experiments is about 50  $\mu$ m. For the generation of shock waves the energy of high explosives (HE) is used, therefore experimental targets are placed within the explosive containment chamber that is certified for the use of up to 100 g of HE in TNT equivalent. The results of latest experiments are presented, including results on explosion and detonation of pressed and emulsion high explosives, shock-induced dense non-ideal plasma of argon and xenon and shock loading of non-uniform metal surfaces.

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 $<sup>^{2}</sup>ITEP$ 

**I6**: Tuesday 11.09.2012, 11:00 - 11:30

# Examining the interior structure of transiting extrasolar giant planets

J.J. Fortney <sup>1</sup>

Transiting exoplanets are those that pass directly in front of their parents stars, allowing us to measure their radii. In particular we have now reached the point in studying transiting planets that we can begin to examine the Jupiter-class planets as a class of astrophysical object. The long-suggested promise of transiting planets is now being realized, in that we can infer the interior structure of planets from a measurement of their mass and radius. We point out that there is an emerging population of planets that are modestly cooler than "hot Jupiters" ( $T_{\rm eff} < 1000~{\rm K}$ ) for which it is relatively straightforward to understand their composition. We have searched this cool group for correlations, and we find several interesting properties regarding the amount of heavy elements within these planets. This sample helps us to understand the structure of Jupiter and Saturn in the context of the composition of their extrasolar planetary "cousins."

<sup>&</sup>lt;sup>1</sup> University of California, Santa Cruz

**T16**: Tuesday 11.09.2012, 11:30 - 11:50

#### Jupiter as an ideal planet to study non-ideal plasmas

<u>Nadine Nettelmann</u><sup>1</sup>, Martin French<sup>1</sup>, Winfried Lorenzen<sup>1</sup>, Andreas Becker<sup>1</sup>, Bastian Holst<sup>2</sup>, Ronald Redmer<sup>1</sup>

Our understanding of giant planets such as Jupiter is strongly dependent on our knowledge about the non-ideal behavior of light elements (e.g., H, He) under high pressures. We present models for Jupiter's internal structure that meet the observational constraints and discuss them in dependence on the physics of Jupiter's main components H and He as predicted from ab initio simulations. In particular, we investigate the influence of the nonmetal-to-metal transition of hydrogen on the transport properties (thermal and electric conductivity) in Jupiter [1], and the helium depletion of Jupiter's atmosphere as a consequence of H-He demixing in the interior. Our models suggest that Jupiter's envelope is separated into two or more layers, and that its core is small [2]. Looking forward to the next generation of space missions such as Juno, we show how current Jupiter models, and hence the assumed behavior of non-ideal hydrogen-helium-water plasmas, can be validated by means of planned astrophysical observations [2].

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<sup>&</sup>lt;sup>2</sup>CEA Arpajon, F-91297, France

<sup>[1]</sup> M. French, A. Becker, W. Lorenzen, N. Nettelmann, M. Bethkenhagen, J. Wicht, R. Redmer, Astrophys. J. Suppl. S. 205, 5 (2012).

<sup>[2]</sup> N. Nettelmann, A. Becker, B. Holst, R. Redmer, Astrophys. J. 750, 52 (2012)

**T17**: Tuesday 11.09.2012, 11:50 - 12:10

# Thermonuclear fusion in dense stars: Electron screening and conductive cooling effects

A.Y. Potekhin<sup>1</sup>, G. Chabrier<sup>2</sup>

We study the plasma correlation effects on nonresonant thermonuclear reactions of carbon and oxygen in the interiors of white dwarfs and liquid envelopes of neutron stars.

We examine the effects of electron screening on thermodynamic enhancement of thermonuclear reactions in dense plasmas beyond the linear mixing rule. Using these improved enhancement factors, we calculate carbon and oxygen ignition curves in white dwarfs and neutron stars. The energy balance and ignition conditions in neutron star envelopes are evaluated, taking their detailed thermal structure into account. The result is compared to the simplified "one-zone model", which is routinely used in the literature. We also consider the effect of strong magnetic fields on the ignition curves in the ocean of magnetars.

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**T18**: Tuesday 11.09.2012, 12:10 - 12:30

#### SAHA-S – thermodynamic model of solar plasma

<u>Gryaznov Victor K.</u><sup>1</sup>, Iosilevskiy Igor L., <sup>2</sup>, Fortov Vladimir E.<sup>2</sup>, Starostin Andrey N.<sup>3</sup>, Roerich Vitali C <sup>3</sup>, Baturin Vladimir A.<sup>4</sup>, Ayukov Sergey V.<sup>4</sup>

SAHA-S thermodynamic model for weakly coupled multi-component plasma of the Sun is represented. The model is based on the basis of chemical picture and takes into account Coulomb interaction of charged particles with exchange and diffraction corrections, relativistic effects and pressure of radiation. Thermodynamic functions of solar plasma were calculated in the range of densities and temperatures typical for the Sun from its surface to the interior. Extended element composition concluded hydrogen, helium and heavy elements from carbon to iron was considered with various heavy element abundance. Component composition concluded atoms, diatomic molecules, electrons and ions from singly charged to nuclei. The last version of the model concluded more than 140 components.

Contribution of various plasma effects in particular effects of interparticle interaction, relativistic effects and pressure radiation effects are considered and analyzed. Comparison of obtained results with other models and results of helioseismic inversion are presented and discussed.

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**17**: Tuesday 11.09.2012, 14:00 - 14:30

### X-ray studies of warm and dense matter

R. Falcone<sup>1</sup>

I will describe three studies of warm and dense matter which use a variety of pump and probe techniques. (1) We use ultrafast optical laser pulses to isochorically heat a solid, which is then probed by ultrafast techniques using synchrotron radiation; this technique reveals the near edge absorption structure of the material and thus the dynamic electronic density of states and electron dynamics. (2) Also, we have used powerful nanosecond laser pulses to drive shocks that compress and heat matter, which is then probed by x-ray plasma backlighter line sources using the inelastic process of Thomson scattering; this technique reveals the electron and ion densities and temperatures. (3) Finally, we use a short pulse x-ray free electron laser to isochorically heat and excite a dense plasma, and we then observe fluorescence and line emission from various ionization stages; this technique reveals novel pathways for plasma and high ionization stage production, and properties of the dense plasma.

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**T19**: Tuesday 11.09.2012, 14:30 - 14:50

## Ultrafast transitions from solid graphite to plasma states induced by x-ray free-electron laser puls

T. Döppner<sup>1</sup>, S.P. Hau-Riege<sup>1</sup>, J.A. Bradley<sup>1</sup>, S.H. Glenzer<sup>1</sup>, C. Fortmann<sup>1</sup>, A. Graf<sup>1</sup>, R. London<sup>1</sup>, J. Krzywinski<sup>2</sup>, M. Frank<sup>1</sup>, K. Sokolowski-Tinten<sup>3</sup>

We used photon pulses from the LCLS x-ray free-electron laser at 2 keV to study ultrafast x-ray-induced transitions of graphite from solid to liquid and plasma states. This was accomplished by isochoric heating of graphite samples and simultaneous probing via diffuse scattering at high time resolution using pulse widths ranging from 40 to 800 fs. From the strong increase of elastic scattering at small angles with pulse length we infer that the disintegration of the crystal lattice and ion heating of up to 5 eV occur within tens of femtoseconds at an intensity of  $2 \cdot 10^{16}$  W/cm<sup>2</sup> [1]. The disintegration of the lattice structure is going along with a change of the inelastic scattering spectra. A comparison to scattering spectra of cold samples obtained at APS, Argonne, supports an ultra-fast structural transition from a highly oriented pyrolytic graphite to amourphous carbon.

[1] S.P. Hau-Riege, A. Graf, T. Döppner et al., accepted for publication in Phys. Rev. Lett. (2012).

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<sup>&</sup>lt;sup>3</sup> University Duisburg-Essen

**T20**: Tuesday 11.09.2012, 14:50 - 15:10

## Probing dense plasmas by x-ray scattering and spectroscopy at European XFEL

<u>Thomas Tschentscher</u><sup>1</sup>, Friedhelm Bell<sup>2</sup>, Marion Harmand<sup>3</sup>, Sven Toleikis<sup>3</sup>

Investigation of solid-density matter under extreme conditions of temperature, pressure, or density and using intense x-ray free-electron laser radiation enables new insight for structural and dynamical properties of these systems. Hard x-ray radiation in the regime up to 5-20 keV is particularly suited due to its high penetration power. We discuss in this paper the application of inelastic x-ray scattering and of x-ray absorption spectroscopy techniques for the investigation of free and bound electrons in highly excited solid and dense plasma systems. The application of inelastic scattering, in particular in the Compton regime, provides model free access to fundamental parameters such as free electron temperature and density. Analytical profiles are shown that can be applied to analyse Compton profiles measured from plasma states including bound and free electrons of arbitrary degeneracy. Furthermore a detailed analysis of the experimental profiles can measure the ionization state of the plasma, at least for low Z systems. We discuss in this context the complementary application of x-ray absorption spectroscopy to investigate the bound electron states inside the plasma in terms of electron temperature.

Since the above discussed techniques depend on ultrashort interaction with the plasma volume they do intrinsically allow for ultrahigh time-resolution enabling to investigate the formation of the equilibrated plasma state following excitation from the unperturbed, cold solid state. Hard x-ray free-electron laser sources do provide the intensity, collimation and bandwidth to perform these studies. A few case studies will be introduced and the implementation of a corresponding experimental station at the European XFEL will be briefly described.

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**T21**: Tuesday 11.09.2012, 15:10 - 15:30

# Properties of hydrodynamic stable non-ideal plasma obtained via X-ray heating of low density foams

Olga N. Rosmej<sup>1</sup>

The unique combination of a Petawatt High-Energy Laser System for Ion beam eXperiments – "Phelix" (Nd:glass) and heavy ion beams of the UNILAC accelerator at Gesellschaft für Schwerionenforschung, Darmstadt, Germany allows investigation of the heavy ion stopping in dense laser produced plasmas. In order to gain high degree of homogeneity and approach plasma with a coupling parameter  $\sim 0.5-1$  a combined hohlraum-target concept have been investigated, where the cold matter is heated volumetrically by means of X-rays generated in the gold hohlraum. The application of low density CHO-foam layers for plasma production has demonstrated very high hydrodynamic stability and uniformity of plasma compared to the solid density foils of the same areal density, which expands after heating in sub-nanosecond time scale creating plasma with high temperature and density gradients. Results of experiments carried out at GSI-Darmstadt and PALS-laser facility in Prague will be presented, where a wide variety of diagnostic methods have been applied. Measurements on the thermal wave propagation, opacity, self-radiation and heavy ion-stopping properties of plasma heated by means of soft X-ray hohlraum radiation will be discussed. Numerical simulations of hydrodynamic and radiation properties of high density CHO-plasma show good agreement with experimental results.

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**18**: Tuesday 11.09.2012, 16:00 - 16:30

### Effective interactions and ion dynamics in warm dense matter

D.O. Gericke<sup>1</sup>, J. Vorberger<sup>1</sup>, I.M. Tkachenko<sup>2</sup>, Z. Donko<sup>3</sup>

The combination of strong forces between the ions, degenerate electrons and the possibility of bound states makes warm dense matter hard to describe. Moreover, the complex interaction of electrons and ions gives rise to a short-range structure in the ionic subsystem that, in turn, determines many other properties of the system. Ab initio simulations, like DFT-MD, are a possible approach to study the equilibrium physics of such complex systems and have been successfully applied to obtain the static ion structure factor. However, present DFT-MD simulations cannot yield the ion dynamics as the simulated time is too short to cover all aspects of the ion motion. On the other hand, classical MD simulation of the ions can be run long enough to obtain dynamic structure factors for a given interaction.

In this contribution, we will show how quantum and classical techniques can be combined to calculate the dynamics of the ion structure in warm dense matter. First, several techniques for the extraction of effective ion-ion potentials from DFT-MD simulations are reviewed and discussed. We find that most deviations from the screened Coulomb potential are due to partial ionization. We also recover the known fact that even potentials of a qualitatively different form may yield a similar static structure and conclude that only the dynamic ion structure factor will reveal, in comparison with experiments, the true inter-ionic forces in warm dense matter. To obtain predictions for the ion dynamics, we apply the extracted potentials in classical MD simulations. As expected, the results show significant deviations from simulations using screened Coulomb interactions. We also apply a number of theoretical models, namely static and dynamic local field corrections, Mermin-like functions and the method of moments with local constrains, to calculate the dynamic ion structure factor. The comparison with the simulation data shows that our theoretical understanding of the ion dynamics in complex systems as warm dense matter is far from being sufficient: only theories with, at least, one adjustable parameter can be made to agree well.

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**T22**: Tuesday 11.09.2012, 16:30 - 16:50

#### Thomson scattering on inhomogeneous targets

P. Sperling<sup>1</sup>, D. Bauer<sup>1</sup>, Th. Bornath<sup>1</sup>, T. Liseykina<sup>1</sup>, T. Döppner<sup>2</sup>, C. Fortmann<sup>2</sup>, S.H. Glenzer<sup>2</sup>, G. Gregori<sup>3</sup>, M. Harmand<sup>4</sup>, S. Toleikis<sup>4</sup>, R. Thiele<sup>5</sup>, Th. Tschentscher<sup>6</sup>, R. Redmer<sup>1</sup>

The introduction of free electron lasers enables new pump-probe experiments to characterize warm dense matter, i.e. systems at solid-like densities and temperatures of several eV. For instance, such extreme conditions are relevant for the interior of giant planets and along the compression path of inertial confinement fusion capsules. Due to strong correlations and quantum effects, a theoretical treatment of warm dense matter is rather complicated so that consistent methods of many-body physics have to be applied. Theoretical results for the pair distribution functions and the equation of state can now be checked using new experimental techniques. For instance, within ongoing experimental campaigns, a short-pulse optical laser irradiates targets, e.g. liquid jets (at FLASH) or thin foils (at LCLS), that is subsequently probed with brilliant X-ray radiation. The inhomogeneous plasma prepared by the optical laser is characterized with particle-in-cell simulations. The interaction of the X-ray probe radiation with the inhomogeneous plasma is taken into account for different time delays between pump and probe via radiation hydrodynamic simulations.

For the pump-probe experiments performed on liquid hydrogen (helium) at FLASH, we calculate the respective scattering spectrum based on the Born-Mermin approximation for the dynamic structure factor considering the full density and temperature dependent Thomson scattering cross section throughout the target. We can identify plasmon modes that are generated in different target regions and monitor their temporal evolution. Combining these results with the ion signal, the temperature equilibration between electrons and ions can be studied as well. Therefore, such pump-probe experiments are promising tools to measure not only the important plasma parameters density and temperature but also to gain valuable information about their time-dependent profile throughout the target. The method described here can be applied to various pump-probe scenarios by combining optical lasers, soft and hard X-ray sources.

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**T23**: Tuesday 11.09.2012, 16:50 - 17:10

# Linear plasma response, electrostatic fluctuations and Thomson scattering

W. Rozmus<sup>1</sup>, C. Fortmann<sup>1</sup>, S.H. Glenzer<sup>1</sup>, A.V. Brantov<sup>2</sup>, V.Yu. Bychenkov<sup>2</sup>

A nonlocal and nonstationary transport theory provides a method of solution of the initial value problem for the full set of linearized Fokker-Planck kinetic equations with Landau collision operators. The closure relations reduce the problem of finding particle distribution functions to the solution of the close set of fluid equations. This has been recently realized for the electron-ion plasma in the entire range of particle collisionality [1]. We will discuss new complete results for  $\epsilon(k,\omega)$  in electron-ion plasmas. The full description of the longitudinal plasma response is used in the derivation of damping and dispersion relations for electrostatic fluctuations such as Langmuir waves, ion-acoustic and entropy modes. Particle collision effects are rigorously accounted for. The Onsager's regression of fluctuations method is applied to derive dynamical form factor  $S(k,\omega)$  and Thomson scattering (TS) cross-section from the set of fluid equations. The new theory of  $S(k,\omega)$  is a generalization of the previous results [2] by including high frequency, plasma fluctuations and zero frequency entropy modes. Our results provide rigorous limiting expressions for different theories of the TS cross-sections in dense strongly coupled plasmas [3]. We will examine the importance of an entropy mode peak as the direct measure of ion temperature in TS experiments.

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<sup>[1]</sup> A.V. Brantov, V.Yu. Bychenkov, W. Rozmus, Phys. Rev. Lett. in press (2012); Zhen Zheng, W. Rozmus, V. Yu. Bychenkov, et al. Phys. Plasmas 16, 102301 (2009).

<sup>[2]</sup> J.F. Myatt, W. Rozmus, V.Yu. Bychenkov et al. Phys. Rev. E 57, 3383 (1998).

<sup>[3]</sup> S.H. Glenzer, R. Redmer, Rev. Modern Physics 81, 1625 (2009).

**T24**: Tuesday 11.09.2012, 17:10 - 17:30

## The extended Mermin approximation for the collisional plasma dielectric function

Yu.V. Arkhipov<sup>1</sup>, A.B. Ashikbaeva<sup>1</sup>, A.E. Davletov<sup>1</sup>, <u>I.M. Tkachenko</u><sup>2</sup>

Mathematical properties of the Mermin and the local-field-corrected Mermin model approximation for the collisional plasma dielectric function are analyzed within the method of moments. Some advantages and drawbacks of the Mermin formula and their consequences for the calculation of the plasma stopping power are pointed out. The prolongation of the plasma dielectric function in the random-phase approximation onto the complex frequency upper half-plane is obtained and studied as well.

This work was partially supported by the Ministry of Education and Science of the Republic of Kazakhstan under Grants No. ITT 02/2012 and IPC 11/2012, and by the Spanish Ministerio de Ciencia e Innovacion under Grant No. ENE2010-21116-C02-02. The authors acknowledge the financial support of KazNU; I. M. T. is grateful to the UPV for the sabbatical leave he was granted and to the KazNU for its hospitality.

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Abstracts of talks Wednesday 12.09.2012, 9:00 - 12:30

**19**: Wednesday 12.09.2012, 9:00 - 9:30

# Extremely high-intensity laser interactions with fundamental quantum systems

Christoph H. Keitel<sup>1</sup>

Laser-driven relativistic quantum dynamics and the key features of quantum vacuum are introduced briefly. Applications such as the characterization of extreme laser pulses are discussed. Then, emphasis is placed on situations where the influence of vacuum fluctuations is shown to become observable with present facilities or those under construction. In the following, pair production is investigated in strong laser fields, especially with the aid of other injected particles. Finally, spin effects and the role of radiative reaction for single particles and in plasmas are presented.

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**T25**: Wednesday 12.09.2012, 9:30 - 9:50

#### Ionization dynamics in laser-irradiated droplets

<u>Tatyana Liseykina</u><sup>1</sup>, Dieter Bauer<sup>1</sup>

Using three-dimensional, relativistic particle-in-cell simulations with ionization included we study the ionization dynamics and plasma formation in intense laser-droplet interaction. The numerical simulations show that there exists a broad laser intensity regime for which wavelength-sized targets are not fully ionized in plane-wave incident pulses. For higher-Z material this applies even to ultra-high intensities. Moreover, the results reveal that there exists a range of incidence angles at which oscillating electric fields penetrate into the droplet, ionizing its interior. We attribute this effect to the local field enhancements at the droplet surface that can be calculated using Mie theory. The penetration of the fields into the droplet leads to the formation of a highly asymmetric density distribution in the droplet interior, concentrated mostly in the polarization plane. The higher charge states are thereby not only concentrated within the skin layer close to the surface but also around a focal point in the droplet interior. The ionization dynamics in the case of focused laser pulses depends on the position of the focal spot and is also discussed.

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**T26**: Wednesday 12.09.2012, 9:50 - 10:10

### A wide-range model of intense laser interaction with matter

N.E. Andreev<sup>1</sup>, K.V. Khishchenko<sup>1</sup>, O.F. Kostenko<sup>1</sup>, P.R. Levashov<sup>1</sup>, M.E. Povarnitsyn<sup>1</sup>, O. Rosmej<sup>2</sup>, M.E. Veysman<sup>1</sup>

A wide-range model is used for the description of material response on ultrashort laser action. The model is developed on the basis of two-temperature hydrodynamics with heat transport, ionization, plasma expansion, electron-ion collisions and twotemperature equation of state for an irradiated substance. Comparison of experimental findings with the results of simulation is used both for the numerical model verification and for calculation of plasma thermodynamic parameters that cannot be measured directly in experiment. For relativistic intensities of the main pulse, even high-contrast beams can produce plasma on the target surface due to a long nanosecond prepulse action which results in an undesirable early smearing of the target. In particular, dynamics of thin foils under the prepulse action is especially important for the laser ion acceleration technique and the promising target design for efficient X-ray generation. To avoid the influence of the long laser prepulse a thin foil can be arranged in front of the target. The analysis of the multi-stage foil dynamics is performed using a wide-range two-temperature hydrodynamic model, which correctly describes the foil expansion starting from the normal solid density at room temperature. Simulations show that varying the foil thickness one can diminish the prepulse transmission through the foil material in many orders of magnitude and at the same time provide the total transparency of the foil plasma by the moment of the main high-intensity ultra-short pulse arrival. Modeling of shielded and unshielded target dynamics demonstrates the effectiveness of this technique. However, the prepulse energy re-emission by the shielding foil plasma can be sizable producing an undesirable early heating of the target placed behind the foil. The generation of characteristic X radiation under vacuum heating of electrons at the surface of a massive target by a p-polarized high contrast femtosecond laser pulse is considered.

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T27: Wednesday 12.09.2012, 10:10 - 10:30

## Quantum plasma simulations beyond the semiclassical approximation

H.-J. Kull<sup>1</sup>

<sup>1</sup>RWTH Aachen</sup>

Weakly coupled degenerate electron plasmas are of fundamental importance in high energy density physics (HEDP) with important applications in high-intensity laser-matter interaction and in inertial confinement fusion (ICF). The basic quantum kinetic equation for the electron dynamics in dense plasmas is the quantum Vlasov equation. In the semiclassical approximation it reduces to the classical Vlasov equation corrected by quantum potentials. Plasma simulations are conveniently performed by the classical particle-in-cell (PIC) approach with appropriate quantum-potentials.

In the present work, we consider the kinetic treatment of dense quantum plasmas beyond the semiclassical approximation[1]. Carrier envelope waves (CEW) are introduced as representative quantum states. The phase of the carrier wave can be chosen to satisfy the classical Hamilton-Jacobi equation. The amplitude satisfies a Schrödinger-type equation for the electron density along classical trajectories. In the classical limit this equation is just the continuity equation. Solving the quantum-mechanical Schrödinger equation or the classical continuity equation coupled to the Hamilton-Jacobi equation and the Poisson equation provides an alternative approach to plasma simulations. It is based on the exact physical particle density and allows one to generalize the method from the classical to the quantum regime without further approximations. Plasma waves and electron-ion collisions in dense quantum plasmas will be studied by this method.

[1] A. Schmidt-Bleker, W. Gassen, and H.-J. Kull, Nonlinear plasma waves and wavebreaking in quantum plasmas, EPL 95, 55003 (2011).

**I10**: Wednesday 12.09.2012, 11:00 - 11:30

#### Physics of liquid-phase dusty plasmas

#### John Goree<sup>1</sup>

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A dusty plasma is a four-component mixture of electrons, ions, neutral gas atoms, and small particles of solid matter. In astronomy, the solid particles are called dust particles, and so the mixture is called a dusty plasma. The dust particles constantly collect electrons and ions, but they collect more electrons than ions, so that they gain a negative electric charge. In laboratory experiments, this charge can be as large as ten thousand electronic charges, for a particle of several microns in diameter.

Because of this large charge, the mutual repulsion between particles has a potential energy that can easily exceed the particle kinetic energy. Thus, the dust particles are strongly coupled, even if the electrons and ions are not. In an experiment, the motion of individual dust particles can be tracked using video microscopy.

In this talk, I will review some experiments and computer simulations of dusty plasmas that behave like a liquid. There is much that can be learned about a liquid by observing the motion of individual particles, as can be done in experiments by tracking particles and in simulations by integrating their equations of motion.

Under thermal conditions, particle motion can be decomposed into a superposition of two kinds of sound waves: compressional and shear. In a liquid, the shear waves can propagate only a limited distance before they are damped, but they nevertheless can be detected. One feature of this propagation is a cutoff in the wavenumber. Only for sufficiently large wavenumbers (small wavelengths) can the wave propagate. The detection of these waves, and the measurement of the cutoff wavenumber, will be one topic of this talk.

The other topic of this talk will be the viscoelasticity of the liquid-phase dusty plasma. Like many soft materials, a simple liquid can both dissipate energy (viscosity) while also storing energy (elasticity). The viscoelastic properties of a liquid are measured by obtaining the wavenumber or frequency-dependent viscosity. Both experimental and simulation results will be presented.

Work supported by the U.S. National Science Foundation and NASA

**T28**: Wednesday 12.09.2012, 11:30 - 11:50

# Ordering and transport phenomena in strongly coupled systems of charged dust in traps and plasmas

Oleg F. Petrov<sup>1</sup>

The problems associated with the transport phenomena in dissipative systems of interacting dust particles are of significant interest in various fields of science and technology. The transport coefficients are fundamental parameters that reflect the nature of the inter-particle potentials, and the phase state of the systems.

A characteristic feature of dusty plasmas is the strong interaction between dust particles, which may lead to the formation of ordered liquid-like and crystallike structures that may be considered as macroscopic strongly coupled Coulomb systems (SCCS). One of the central problems associated with experimental studies of stable SCCS is that of ensuring the levitation of charged particles.

In the present work dust structures are studied experimentally in dc glow discharge plasmas in mixtures of "light" and "heavy" gases (helium and krypton). Characteristic feature of the dusty plasma structures observed was the formation of linear, chain-like dust structures with strong grain—grain interaction in the ion drift direction. The results of simulations performed for a mixture containing a "heavy", easily ionized gas suggest a strong effect of gas composition on dust structure formation in discharge plasmas.

Dense dust structures in a dc glow discharge are considered at gas cryogenic temperatures (LN2 and LHe). Results on the experimental investigations of new phenomenon of cryogenic "spheroidizing" were presented. The "spheroidizing" is process of the dust structure transition to compact globular (spherical) shape at cryogenic temperatures. Experimental study of the kinematic viscosity has been carried out for dust particles of different sizes in weakly ionized plasma. Results of measurements of viscosity for weakly correlated dusty-plasma systems in a wide range of coupling parameters are presented. Comparison of the measured viscosity constants with the theoretical estimations and the numerical data are presented.

An original method for the simultaneous recovery of the interparticle interaction potential and the electrostatic confining potential in plasma-dust systems has been developed. The method is based on solving the inverse problem, which describes particle motion by system Langevin equations.

This work was supported by the Research Program of the Presidium of the Russian Academy of Sciences "Matter under High Energy Densities" and by the Russian Foundation for Basic Research, Project No. 10-02-01428.

<sup>&</sup>lt;sup>1</sup> Joint Institute for High Temperatures RAS

**T29**: Wednesday 12.09.2012, 11:50 - 12:10

# Dust acoustic waves in non-equilibrium plasmas at elevated pressure

A.V. Filippov<sup>1</sup>, <u>A.N. Starostin</u><sup>1</sup>, I.M. Tkachenko<sup>2</sup>

Dielectric properties of dusty plasmas are studied on the basis of the hydrodynamic (HD) approach and within the non-perturbative moment approach for the bi-Yukawa interaction potential with different screening constants. The results obtained within these approaches are shown to be in good agreement at low wave numbers. The hydrodynamic approach is applicable only in the long-wavelength approximation, but the moment approach does not have such restrictions. Thus the latter allows us to study dielectric properties of dusty plasmas at higher values of both the wavenumber and the nonideality parameter.

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**T30**: Wednesday 12.09.2012, 12:10 - 12:30

### Anomalously high dust particle charging by an electron beam

S.I. Kopnin<sup>1</sup>, T.I. Morozova<sup>1</sup>, S.I. Popel<sup>1</sup>

The existence of anomalously high negative dust particle charges has been shown in the experiments on dust particle charging by an electron beam [1]. Here, we develop a theory allowing us to explain the values of dust particle charges in these experiments. For this purpose we take into account the field emission current in addition to the electron beam current on a dust particle. The field emission is associated with the quantum tunnel effect of atomic particles through some potential barriers. External electric field (related to dust particle charging) reduces this barrier (the so-called Schottky effect). Thus when the dust particle charge is growing, the potential barrier is reducing. Theoretical results obtained are in a good accordance with the experimental data [1].

This work is supported by the Presidium of the Russian Academy of Sciences (the basic research program No. 22 "Fundamental problems of research and exploration of the solar system"), the Division of Earth Sciences of the Russian Academy of Sciences (the basic research program "Nanoscale particles: conditions of formation, methods of analysis and recovery from mineral raw"), and the Russian Foundation for Basic Research (grant No. 12-02-00270-a).

[1] M.N. Vasil'ev, N.A. Vorona, A.V. Gavrikov, O.F. Petrov, V.S. Sidorov and V.E. Fortov, Techn. Phys. Lett. 36, 1143 (2010)

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Abstracts of talks Thursday 13.09.2012, 9:00 - 17:30 **I11**: Thursday 13.09.2012, 9:00 - 9:30

## Beyond Landau-Spitzer: Collision rates in strongly coupled ultracold plasmas

Thomas Killian<sup>1</sup>

Ultracold neutral plasmas provide a powerful platform for studying collisional equilibration in strongly coupled systems. They are created by photoionizing laser-cooled atoms at the ionization threshold, and the resulting ion and electron temperatures are orders of magnitude colder than in traditional neutral plasmas. The ions are strongly coupled and equilibrate with Coulomb coupling constant  $1 < \Gamma_i < 4$ . Because the density is relatively low compared to high-density strongly coupled plasmas, all relevant timescales are much longer, which provides great advantages for experiments.

The creation of the plasma involves a rapid hardening, or quench of the particle interactions. This leads to an exchange of potential and kinetic energy during subsequent thermalization called correlation induced heating. This is followed by oscillations of the kinetic energy at the ion plasma oscillation frequency. It is also possible to perturb the velocity distribution in an equilibrium plasma and observe the relaxation to a Maxwell-Boltzmann distribution. This allows a measurement of the collision rate in the strongly coupled regime, beyond the point where standard Landau-Spitzer theory becomes invalid. Both experiments probe general features of equilibrating strongly coupled systems and can be related to dynamics in other laser-produced plasmas.

<sup>&</sup>lt;sup>1</sup>Rice University

**T31**: Thursday 13.09.2012, 9:30 - 9:50

### Nonideal plasmas in a strong magnetic field

<u>Torben Ott</u><sup>1</sup>, Michael Bonitz<sup>1</sup>, Hanno Kählert<sup>2</sup>

We study a strongly correlated one-component plasma with Coulomb and Yukawa interaction in the presence of a strong magnetic field. Such situations are of relevance for trapped ions, dusty plasmas, for the concept of magnetized target fusion, and for the properties of white dwarf stars and for neutron stars.

We present first-principle molecular dynamics simulation results for the transport properties, such as diffusion coefficient [1] and for the collective oscillation spectrum in two [2] and three dimensions [3]. Finally, we discuss how to achieve strong magnetization in strongly correlated laboratory plasma experiments.

- [1] T. Ott, and M. Bonitz, Phys. Rev. Lett. (2011)
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**T32**: Thursday 13.09.2012, 9:50 - 10:10

## Acoustic and optic modes in strongly coupled binary liquids and solids

G.J. Kalman<sup>1</sup>, Z. Donko<sup>1,2</sup>, P. Hartmann<sup>1,2</sup>, K.I. Golden<sup>3</sup>, S. Kyrkos<sup>4</sup>

A theoretical analysis of the acoustic modes of a binary liquid reveals a profound difference between their behavior in the weak coupling and strong coupling phases. In the weak coupling limit the two components interact via the mean field only and the oscillation frequency is governed by the light component. In the strong coupling limit the mode frequency is governed by the combined mass of an average atom [1], where the heavy component dominates. MD simulation of the collective excitations in two- and three-dimensional binary Yukawa systems extend and confirm the theoretical results. In the crystalline solid phase, corresponding to different  $Z_1/Z_2$  and  $c_1/c_2$  ratios, various crystal structures form, which then govern the formation of the optic modes and their survival in the liquid phase. A stability analysis helps to determine the boundary in parameter space between the different structures.

[1] G.J. Kalman, Z. Donko, P. Hartmann, and K.I. Golden, Phys. Rev. Lett. 107, 175003 (2011).

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**T33**: Thursday 13.09.2012, 10:10 - 10:30

# Dynamic shielding, antishielding, cut offs, and the Coulomb paradox

P. Mulser<sup>1</sup>

Dynamic shielding is of particular relevance in stopping of swift ions in matter and in collisional laser beam absorption at high intensities. Traditionally shielding is treated in a linearized approach in Fourier space. The act of a collision of an electron with an ion is an impact-like, high frequency event of delta function character, in contrast to the adiabatic, low frequency interaction. The latter may contribute to diffusion but not to momentum and energy transfer. Subjecting collisions to a Fourier decomposition means to describe a delta function by the superposition of waves of all frequencies and wavelengths and constant amplitude. This may frequently lead to very slowly converging series (10<sup>3</sup> terms and more in presence of strong drifts), erroneous physical interpretation ("closest approach", "minimum impact parameter") and to analytic expressions which are pure mathematical artifacts, e.g., double logarithm in absorption coefficients of laser beams.

By performing the analysis under consideration in position space several of the characteristic difficulties above are circumvented and compact formulas result in which the "cut offs" come about in a natural way, either as the result of correct analysis, or on the basis of physical necessity. An additional advantage is the extension made more direct into the nonlinear domain and the definition of validity of the models.

All aspects are exemplified by the analysis of ion beam stopping and laser light absorption in dense plasmas, the Barkas effect and the solution to the Coulomb paradox.

<sup>&</sup>lt;sup>1</sup> TU Darmstadt

**I12**: Thursday 13.09.2012, 11:00 - 11:30

### Transport properties and equation of states for dense deuteriumtritium plasmas

Cong Wang<sup>1</sup>, Xian-Tu He<sup>1</sup>, and Ping Zhang<sup>1</sup>

Consistent descriptions of the equation of states, and information about transport coefficients of deuterium-tritium mixture are demonstrated through quantum molecular dynamic (QMD) simulations (up to a density of  $600 \text{ g/cm}^3$  and a temperature of  $10^4 \text{ eV}$ ). Diffusion coefficients and viscosity are compared with one component plasma model in different regimes from the strong coupled to the kinetic one. Electronic and radiative transport coefficients, which are compared with models currently used in hydrodynamic simulations of inertial confinement fusion, are evaluated up to 800 eV. The Lorentz number is also discussed from the highly degenerate to the intermediate region.

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**T34**: Thursday 13.09.2012, 11:30 - 11:50

# Constraint-based development of orbital-free free energy density functionals

S.B. Trickey<sup>1</sup>

Predicting real material structures and properties is a demanding task even in the ground state and is far harder for warm dense matter. WDM requires reliable quantum statistical mechanical approximations applicable to systems with multiple ionization states, high overlap of valence and nominal core states, transient exotic molecules, and widely varying local order. Molecular dynamics for the ions with ground-state density functionals for the equilibrium electronic free-energy is the state of the art. The Kohn-Sham solution is the computational bottleneck.

Since the basic DFT theorems (Hohenberg-Kohn, Mermin) are independent of KS, orbital-free DFT (of-DFT) calculations with costs which scale with the relevant system volume should be possible. The challenge is reliable approximate free-energy functionals. Compared to effort on ground-state approximations, progress on of-FE functionals is tiny. The most familiar problem (dating from Thomas-Fermi) is the non-interacting kinetic energy  $\mathcal{T}_s$ . Less obvious is the problem of today's emphasis on explicitly orbital-dependent exchange-correlation functionals  $E_{xc}$ . Then there is proper temperature dependence, including non-interacting entropy functionals. With no mechanical way (e.g. diagrammatic perturbation theory) to construct improved approximations, the primary non-empirical procedure is to impose as many constraints as possible on relatively simple, sensibly designed functional forms. I shall discuss our recent constraint-based development of generalized gradient approximation  $\mathcal{T}_s$ ,  $E_{xc}$ , and noninteracting of-FE functionals. Topics include relevant constraints (positivity, bounds, limits and asymptotics, etc.), identification of appropriate reduced-gradient variables for generalized gradient approximation free energies, choices of functional forms, and some consequences and limitations.

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<sup>&</sup>lt;sup>1</sup>Quantum Theory Project (Physics, Chemistry), Univ. of Florida

**T35**: Thursday 13.09.2012, 11:50 - 12:10

## Simulation of electron propagation in nonideal plasmas using split wave packet molecular dynamics

N.A. Kazeev<sup>1</sup>, I.A. Valuev<sup>1</sup>, <u>I.V. Morozov</u><sup>1</sup>

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The use of electron-ion pseudopotentials in classical molecular dynamics simulations of nonideal plasmas restricts the applicability of this method to high temperatures, high ionization degrees and near equilibrium states. There are several techniques to overcome these limitations [1]. One of them is Wave Packet Molecular Dynamics (WPMD), where electron quantum dynamics is approximated by propagation of wave packets [2], parameterized by a small number of dynamic variables. The exchange interaction between electrons of the same spin in the Hartree-Fock limit can be taken into account using antisymmetrized wave packets [3].

Poor accuracy for electronic bound states at ions and spreading of wave packets for weakly bound electrons are known problems of the existing WPMD models for non-ideal plasmas. We address both issues using a new technique based on multiple Gaussian expansion of the single-electron wave function, which is called Split Wave Packet Molecular Dynamics (SWPMD) [4]. Calculations of the ground state energies of small atoms and molecules show that this method provides better accuracy than the original WPMD. Representing an electron by at least three Gaussians results in the ground state energy for H and He to be within 1% error compared to the exact values.

The main feature of SWPMD is the ability to study electron dynamics taking into account the wave function branching. As a test case we consider tunnel ionization of simple atoms in a short laser pulse. It is shown that the SWPMD results are in a good agreement with more accurate quantum-mechanical calculation methods. Other dynamical events such as elastic and inelastic electron-ion scattering in nonideal plasmas are considered.

In future it is planned to apply the new method to model bound states of electrons and ions in nonideal plasmas and combine it with the classical Coulomb interaction model for free electrons. It is believed that such a combined approach can be used to reduce computational problems related to wave packet spreading.

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<sup>[4]</sup> I.V. Morozov, I.A. Valuev. Contrib. Plasma. Phys. V. 52, P. 140 (2012).

**T36**: Thursday 13.09.2012, 12:10 - 12:30

#### Dynamical properties of nonideal plasma on the basis of effective potentials

T.S. Ramazanov<sup>1</sup>, Zh.A. Moldabekov<sup>1</sup>, S.K. Kodanova<sup>1</sup> *IETP*, Al Farabi Kazakh National University

Microscopic and dynamical properties of a nonideal complex plasma are studied by theoretical and computer simulation methods. In order to describe the interactions between particles several effective potentials are used. These potentials take into account quantum mechanical, screening and polarizations effects in nonideal [1,2] and complex [3,4] plasmas. The computer simulation method was proposed for modeling of microscopic and dynamic properties of nonideal complex plasmas. The peculiarity of this method is the obtaining of dynamic microscopic states of the nonideal plasma without direct integration of equations of motions. The Coulomb logarithm for a dense semiclassical fully and partially ionized plasma was derived. Stopping power and relaxation processes of nonideal plasma were studied on the basis of the Coulomb logarithm. The comparison with data of other theoretical and experimental works was carried out.

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**I13**: Thursday 13.09.2012, 14:00 - 14:30

# Electron energy transport and AC conductivity of nonequilibrium warm dense gold

Andrew Ng<sup>1</sup>

Electron energy transport and AC conductivity are basic properties in which electron screening and ion-ion correlation play an important role. In this talk, I will discuss two recent studies of these properties based on femtosecond laser excitation of 30nm-thick gold foils under isochoric conditions. In the first experiment, simultaneous measurements of front and rear surface reflectivity of the heated foil reveal onset of non-uniform heating when excitation energy flux exceeds  $\sim 7 \cdot 10^{12} \ \mathrm{W/cm^2}$ . This is attributed to flux-limited energy transport driven by non-thermal electrons. In the second experiment, temporal evolution of AC conductivity of the heated foil is determined from simultaneous measurements of reflection and transmission of a chirped probe pulse. The results serve as the first benchmark for testing ab-initio model for self-consistent calculation of equation of state and transport properties of nonequilibrium warm dense matter.

<sup>&</sup>lt;sup>1</sup> University of British Columbia

**T37**: Thursday 13.09.2012, 14:30 - 14:50

# Multiscale Approach to Strongly Correlated Multi-component Plasmas in Nonequilibrium

Patrick Ludwig<sup>1</sup>, Michael Bonitz<sup>1</sup>, Jim Dufty<sup>2</sup>

A key problem in the description of nonideal, multi-component plasmas is the drastic difference in the r,t-scales which prohibits first-principle simulations, in particular in nonequilibrium.

Therefore, we develop a multiscale approach for dense quantum plasmas such as partially ionized Warm Dense Matter, where a full dynamic treatment of the pair correlations of the heavy particles is crucial. To this end, the ions are treated exactly by classical Langevin Dynamics simulations, whereas the electrons are treated fully quantum-mechanically on the basis of a quantum kinetic equation. The coupling of the two is performed in linear response and fully includes the dynamical screening of the ion-ion interaction on the basis of a nonequilibrium extension of the Mermin formula extending our recent results [1,2,3].

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- [2] P. Ludwig, H. Kählert, and M. Bonitz, Plasma Phys. Control. Fusion **54**, 045011 (2012).
- [3] P. Ludwig, W.J. Miloch, H. Kählert, and M. Bonitz, accepted for publication in New J. Phys. (2012); arXiv:1201.1714

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<sup>&</sup>lt;sup>2</sup> University of Florida

**T38**: Thursday 13.09.2012, 14:50 - 15:10

#### Mass transport in warm dense matter conditions

 $\underline{\text{L. Collins}}^1,$  J. Kress $^1,$  F. Lambert $^2,$  C. Ticknor $^1,$  D. Herring $^1,$  L. Burakovsky $^1LANL$   $^2CEA$ 

Large-scale hydrodynamical simulations of fluids and plasmas under extreme conditions require knowledge of certain microscopic properties such as diffusion and viscosity in addition to the equation-of-state. To determine these dynamical properties, we employ quantum molecular dynamical (MD) simulations on large samples of atoms. The method has several advantages: 1) static, dynamical, and optical properties are produced consistently from the same simulations, and 2) mixture properties arise in a natural way since all intra- and inter-particle interactions are properly represented. We utilize two forms of density functional theory: 1) Kohn-Sham (KS-DFT) and 2) orbital-free (OF-DFT). KS-DFT is computationally intense due to its reliance on an orbital representation. As the temperature rises, the Thomas-Fermi approximation in OF-DFT begins to represent accurately the density functional, and provides an efficient and systematic means for extending the quantum simulations from the warm, dense mater regime to very hot conditions. We have performed KS-DFT and OF-DFT calculations of the self-diffusion, mutual diffusion, and shear viscosity for Al, Li, H, and LiH. We examine trends in these quantities and compare to more approximate forms such as the one-component plasma model. We also determine the validity of mixing rules that combine the properties of pure species into a composite result. In addition, we have employed OF-DFT and classical MD techniques to explore non-equilibrium processes involving the mixing of various components at an interface.

**T39**: Thursday 13.09.2012, 15:10 - 15:30

#### Recombination in dense ion plasmas

A. Lankin<sup>1</sup>, <u>G. Norman</u><sup>1</sup>

<sup>1</sup> Joint Institute for High Temperatures RAS

Recombination of ions is important after the electrical breakdown of sulfur hexafluoride and transformer oil, at pulsed-discharge-in-water plasma channel relaxation, at chemical lasers initiation, at discharges in air and other electronegative media. Ion recombination possesses peculiarities which tell it from electron-ion recombination. (a) Collisions of ions with neutral particles are predominant, since the degree of ionization is rather low. (b) As the temperature is also relatively low, complex cluster ions are formed. Both factors (a) and (b) are able to influence the nonideality dependence of the recombination rate. (c) The third particle is not necessary for the recombination since the tunnel transition of the electron from the negative to positive ion can take place when the ions approach to each other. Various combinations of the above mentioned factors result in different mechanisms of the recombination. Pair processes prevail at low densities when ions approach each other along ballistic trajectories. The second mechanism relates to higher densities when three or multi-particle processes dominate the recombination. A transient ion pair is formed and loses its excess energy gradually to the environment. The recombination takes place when the interionic spacing becomes less then the critical one. The mechanism is close to the collisional recombination in the electron-ion plasmas. The effect of the recombination suppression occurs for both electron-ion and ion-ion cases in nonideal plasmas. The reason is that the spectrum domain  $\Delta E$  intermediate between free continuous and low-lying excited pair energy levels exceeds temperature and the one-step jumps across  $\Delta E$  become the limiting recombination mechanism. The third mechanism is diffusion-controlled recombination at high densities. The second mechanism is mostly considered in the paper. Two suppression factors are revealed. Sulfur hexafluoride example shows how increase of  $\Delta E$  with density suppresses recombination for nonideality above 0.3. Ionmolecular clusters turn out to be unstable but ion-molecule interactions increase the  $\Delta E$  value. Fluorine example shows the significance of solvation even for ideal plasmas when  $\Delta E$  does not influence the recombination. The expression is derived which incorporates both suppression mechanisms for multi-component ion plasmas. The results are in a satisfactory agreement with the experimental date available for both sulfur hexafluoride and fluorine.

**I14**: Thursday 13.09.2012, 16:00 - 16:30

### Laser shock experiments for materials of giant planets

Takayoshi Sano<sup>1</sup>

Laser-driven shock compression can generate conditions of extremely high pressure and high temperature, and thus it is recognized as a quite important tool to examine the interior structure of solar and extra-solar planets in laboratory. Using the GEKKO laser system in Osaka University, we are investigating various materials in extreme conditions relevant to giant-planet interiors. Motivated to understand the metallic transition of hydrogen, which is expected to take place in gas giant planets like Jupiter, we have carried out the laser shock compression of cryogenic liquid hydrogen target (Sano et al., PRB,2011). The Hugoniot pressure, density and temperature are successfully obtained at the same time up to 55 GPa by use of the velocity interferometer (VISAR) and optical pyrometer (SOP). In this talk, we will show the details of the hydrogen experiment, and also review our recent results of planetary materials such as forsterite as for rocky core material and water for the interior structure and dynamo of icy giant planets.

<sup>&</sup>lt;sup>1</sup>ILE, Osaka Univ.

**T40**: Thursday 13.09.2012, 16:30 - 16:50

## Ultra-short transient state of metals produced by intense femtosecond EUV laser

<u>Hitoki Yoneda</u><sup>1</sup>, T. Ohashi<sup>1</sup>, S. Nishio<sup>1</sup>, F. Sato<sup>1</sup>, D. Baek<sup>1</sup>, M. Nagasono<sup>2</sup>, T. Togashi<sup>2</sup>, Y. Inubushi<sup>2</sup>, M. Yabashi<sup>2</sup>, T. Ishikawa<sup>2</sup>

Recently developed extreme ultra-violet free-electron lasers selectively produce inner shell ionization of condensed matter. In this excited material condition, electron energy levels are modified rapidly due to the removal of one electron from the inner shell. This means we expect a large change of optical constants even in the EUV wavelength region. After this ionization, fast relaxation process should occur. These include Auger decay and radiation emission and various other slower process such as electron impact ionization. However, up to now, there has been little experimental investigation of these processes. For this investigation, we prepare a jitter-free ultra-broad white light probe system. In this measurement, the optical properties of the transient state can be determined with sub 100 fs resolution and for the entire UV-Visible-IR wavelength region. Up to now, in the case of gold with 55 nm illumination at the intensity of 1013 W/cm<sup>2</sup>, we observed transient states with lifetimes below 100 fs. The dispersion of the complex dielectric constants shows this is not a simple free-electron feature and we consider that there is some localization of EUV excited electrons. After about 200 fs, the optical properties reach a quasi-steady-state condition, which gradually changes in time. Even in this condition, it is very difficult to explain the measurement with a simple Drude-law free electron response.

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**T41**: Thursday 13.09.2012, 16:50 - 17:10

#### Ionization of atoms by intense attosecond pulses

V.P. Krainov<sup>1</sup>, A.V. Gets<sup>1</sup>

Ionization of atoms by ultrashort few-cycle electromagnetic pulses is considered. First-order time-dependent perturbation theory for the derivation of ionization probability by pulses with different profiles is used. Numerical calculations for hydrogen and xenon atoms are done. Strong field-phase dependence of ionization probability is shown. The ionization probability of atoms by a few-cycle attosecond electromagnetic pulse depends significantly on the shape of the pulse (in particular, whether it is a sine-type or cosine-type pulse). With smooth pulses ionization probability is much greater for cosine-type pulses than for sine-type pulses. It is shown that discontinuity of the derivative of the pulse profile leads to a significant rise in the photoionization probability at fixed pulse energy.

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Abstracts of talks Friday 14.09.2012, 9:00 - 12:10 **T42**: Friday 14.09.2012, 9:00 - 9:20

## Ion beam driven high energy density physics studies at FAIR at Darmstadt

N.A. Tahir<sup>1</sup>, A. Shutov<sup>2</sup>, A.R. Piriz<sup>3</sup>, Th. Stoehlker<sup>1</sup>

Intense heavy ion beams have emerged as a new, very efficient tool to generate High Energy Density (HED) Matter including Warm Dense Matter (WDM) and non-ideal plasmas. A new huge accelerator named, Facility for Antiprotons and Ion Research (FAIR) at Darmstadt, has now entered into construction phase. This facility includes building of a very powerful heavy ion synchrotron, SIS100, that will deliver a bunched intense beam of all stable species of particles from protons up to uranium. During the past 15 years, have carried out extensive theoretical work to assess of the potential of the SIS100 beam to perform research in the field of HED physics in the parameter space that has not yet been accessed with the traditional methods. Several novel experiment designs have been proposed including study of the Equation-of-State of HED matter, research on planetary physics, study of hydrodynamic instabilities and study of material properties of solids under extreme pressures. An overview of this work is presented in this talk.

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<sup>&</sup>lt;sup>3</sup> UCLM, Ciudad Real, Spain

**T43**: Friday 14.09.2012, 9:20 - 9:40

### He-like effective interactions for WDM plasmas

C. Deutsch<sup>1</sup>, H. Rahal<sup>1</sup>, M.M. Gombert<sup>1</sup>

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Present intense efforts dedicated to investigations of WDM properties require the use of accurate pseudoclassical electron-partially stripped ion effective interactions for matter densities in the solid state range and  $T_e \sim 1-10$  eV. So, one has to fill a gap between currently used H-like pseudopotentials and TF ones valid for heavy ions  $(Z\gg 1)$ . Toward this goal,we investigate an extension of the polarization model [1] including spin dependence for the overall wave function (w.f)[2] involving the polarization core (Z-nucleus with 1s electron) and the optical electron interacting strongly with surrounding plasma free particles.

These w.f retain a hydrogenic analytic form supplemented by a quantum defect for l=1 and 2. Ground state is given a multiparametric expression [3]. Canonical pair electron-ion distributions include bound and scattered states, as well. Effective interactions are deduced from them and contrasted to their H-like homologs. The Helike/H-like discrepancy appear very significant for WDM plasmas. This discrepancy steadily decreases with increasing Z and  $T_{\rm e}$ . Applications to canonical thermodynamics are envisioned.

- [1] C. Deutsch, Phys. Rev. A 2, 43 (1970), A 3,1516 (1971) and A 13, 2311 (1976)
- [2] H. Rahal and M.M. Gombert, J. Phys. B 30, 4695 (1997)
- [3] E. Clementi and C. Roetti, At. and Nucl. Data Tables 14, 177 (1974)

**T44**: Friday 14.09.2012, 9:40 - 10:00

### A Resolved-Super-Transition-Arrays method for calculation of the spectral absorption coefficient in hot plasmas

G. Hazak<sup>1</sup>, Y. Kurzweill<sup>1</sup>

A new method, 'Resolved-Super-Transition-Arrays', for calculation of the spectral absorption coefficient in hot plasmas is presented. The formulae of the traditional Super-Transition-Arrays method [1] are recovered from the formulae of the new method by an approximation based on a cumulant expansion truncated at the third term. In the new method an expression for the many-electron two-time dipole autocorrelation function of ions in hot dense plasmas in terms of Complex Pseudo Partition Functions is derived. The Fourier transform with respect to time together with the fluctuationdissipation theorem yields an expression for the spectral absorption coefficient. In this expression a multitude of Gaussian Super-Transition-Arrays sharing the same set of one-electron solutions, required by the traditional method to resolve the detailed spectrum, is replaced by a single Complex Pseudo Partition Function which represents the exact analytical sum of the contributions of all relevant transition arrays. A new computer program is presented, capable of evaluating the absorption coefficient by both the new and the traditional Super-Transition-Arrays methods. A numerical example of gold at temperature 1 keV and density 0.5 g/cm<sup>3</sup>, is presented, demonstrating the simplicity, efficiency and accuracy of the new method.

[1] A. Bar Shalom, J. Oreg, W.H. Goldstein, D. Shvarts and A. Zigler, Phys. Rev. A 40, 3183 (1989)

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**T45**: Friday 14.09.2012, 10:00 - 10:20

## Anomalous diffusion on the basis of the extended master equation

A.A. Dubinova<sup>1</sup>, G.J.F. van Heijst<sup>2</sup>, <u>P.P.J.M. Schram</u><sup>2</sup>, S.A.Trigger<sup>3</sup>

A more general quasi Fokker-Planck is derived to describe particle kinetics in situations where the usual Fokker-Planck equation is not applicable. The obtained equation is valid for arbitrary values of the momentum transferred in a collision and for an arbitrary mass ratio of the interacting particles. The only assumption concerns the smallness of the typical velocity of the particles undergoing diffusion compared to the typical velocity of the background particles. On the basis of the derived equation anomalous diffusion in velocity space is considered for hard-sphere and Coulomb collisional models. In these examples of anomalous diffusion the ambient particles are assumed to have a power type velocity distribution function. In general, the approach developed in this way is another tool for the treatment of anomalous diffusion avoiding the method of fractional differentiation, which is conventional in such problems.

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<sup>&</sup>lt;sup>3</sup> Joint Institute for High Temperatures, Russian Academy of Sciences

**T46**: Friday 14.09.2012, 10:50 - 11:10

## Fully microscopic analysis of laser-driven plasmas via microscopic particle-in-cell simulations (MicPIC)

Christian Peltz<sup>1</sup>, Charles Varin<sup>2</sup>, Thomas Brabec<sup>2</sup>, <u>Thomas Fennel</u><sup>1</sup>

The physics of laser-driven solid-density plasmas is a fundamental problem in modern laser science. A central obstacle in modeling their dynamics is the enormous gap between the physical scales relevant for microscopic and macroscopic phenomena. Microscopic processes, such as the atomic scale microfield dynamics and collisions, require Angstrom resolution, while the macroscopic scale of collective and wave propagation phenomena is of the order of the laser wavelength. Recently, the microscopic particlein-cell (MicPIC) concept has been developed to bridge these microscopic and macroscopic realms of laser-driven plasma physics [1]. MicPIC enables the direct simulation of strongly-coupled plasmas under the inclusion of electromagnetic wave propagation and allows the investigation of processes that have been inaccessible to rigorous numerical scrutiny so far. This will be illustrated by two main findings of our analysis of pre-ionized, resonantly laser-driven clusters. In the linear response regime, MicPIC data is used to determine the individual microscopic contributions to the dielectric cluster response function, such as surface and bulk collision frequencies. The capacity to determine the microscopic underpinning of optical material parameters opens new avenues for modeling nano-plasmonics and nano-photonics systems [2]. In the nonperturbative regime, our analysis reveals an attosecond plasma wave dynamics in laser driven clusters. This opens a new research direction for the field of attosecond science.

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<sup>&</sup>lt;sup>2</sup>Department of Physics, University of Ottawa, Ontario, Canada

<sup>[1]</sup>C. Varin et al., Phys. Rev. Lett. 108, 175007 (2012)

<sup>[2]</sup>C. Peltz et al., submitted

**T47**: Friday 14.09.2012, 11:10 - 11:30

## Electronic correlations in nanoclusters - Molecular dynamics simulations

Mathias Winkel<sup>1</sup>, Paul Gibbon<sup>1</sup>

With the recent developments in experimental possibilities in the field of creation and diagnostics of metallic nanoclusters, the exploration of their interaction with the radiation field gained some importance during the last few years.

Since the quasi free electrons inside the cluster are confined to a very small volume, their collective properties significantly change in comparison to bulk matter. Extending earlier simulations of Raitza et al. [1], we examine optical properties of laser-excited nanoclusters. In particular, we study electronic correlations in a sodium-like material. To cover a broad range from nano- to microscale, the momentum autocorrelation function is evaluated in classical molecular dynamics simulations for systems with less than 200 up to few million electrons. Therefore, we utilize our highly scalable parallel Barnes-Hut tree code PEPC that has been developed at JSC [2].

First results for electronic resonances in metallic nanoclusters are shown and compared to the respective bulk properties.

- [1] T. Raitza et al., Phys. Rev. E 84 (2011), 036406
- [2] M. Winkel et al., Comp. Phys. Comm. 183 (2012), 880

<sup>&</sup>lt;sup>1</sup> Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH, D-52425 Jülich

**T48**: Friday 14.09.2012, 11:30 - 11:50

### Inverse bremsstrahlung heating in noble gas clusters irradiated by femtosecond laser pulses

M. Moll<sup>1</sup>, Th. Bornath<sup>2</sup>, M. Schlanges<sup>1</sup>, V.P. Krainov<sup>3</sup>

In the interaction of atomic clusters with intense laser pulses, nanoplasmas with high density and high temperature are created. Laser energy is absorbed by the free electrons in the cluster nanoplasma via electron-ion collisions. This inverse bremsstrahlung (IB) heating plays an important role for the laser-cluster evolution. In many approaches for the calculation of the IB heating rate such as the Born approximation, large-angle scattering events are underestimated. However, rescattering events of an electron on the same ion play an important role because they increase the amount of energy exchanged between the electrons and the laser field. Further, in noble gas plasmas the electron-ion interaction is often considered for point-like particles. But in particular for the heavier noble gas ions, the electron-ion interaction deviates from point-like particle interaction. This makes it important to take into account not only the screening by the surrounding plasma medium but also the inner structure of the ions what can be accomplished by the use of appropriate model potentials. In the Born approximation, the consideration of the atomic nucleus and the bound electrons changes the IB heating rate drastically. However, for many experimental conditions, the applicability of the Born approximation is questionable.

We present new results [1] for the IB heating rate obtained from a classical approach based on the simulation of individual electron trajectories including multiple scattering of an electron on the same ion where the interaction potential accounts for the inner ionic structure. For Xe and Ar clusters with different degree of ionization, the energy gain of an electron in a single collision is analyzed in detail as a function of various initial parameters such as the laser field phase, the impact parameter, or the field direction. The dependence of the heating rate on the angle between the momentum of the incoming electron and the electric field vector is investigated. Heating rates for the scattering on atomic ions are compared to the scattering on point-like charges. It shows that especially for higher energies and larger nuclear charges of the ions, the consideration of the ionic structure increases the heating rate. The Born approximation, however, overestimates this effect.

[1] M. Moll, Th. Bornath, M. Schlanges and V.P. Krainov, Phys. Plasmas 19, 033303 (2012)

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<sup>&</sup>lt;sup>2</sup> Universität Rostock

<sup>&</sup>lt;sup>3</sup>Moscow Institute for Physics and Technology

**T49**: Friday 14.09.2012, 11:50 - 12:10

## Response of excited nano plasmas due to collective electron dynamics

<u>Thomas Raitza</u><sup>1</sup>, Johannes Höller<sup>1</sup>, Eckhard Krotscheck<sup>1</sup> <sup>1</sup>JKU Linz

The importance of interaction phenomena of nano plasmas with external fields increased due to modern applied technologies such as nano-antennas and transformation optics. Dielectric properties of laser irradiated clusters of  $10^{13}$  -  $10^{16}$  W cm<sup>-2</sup> change dramatically with the size up to a bulk plasma. Besides the Mie resonance multiple complex damped modes appear, see Kresin *et al.* [1], which are just rarely discussed. Simulation results of electrons in metallic clusters up to  $10^3$  atoms will be presented which are in local thermal equilibrium (LTE) after laser excitation [2]. For high temperatures, a restricted molecular dynamics (RMD) scheme was introduced to discuss the resonance frequencies of the classical collective electron dynamics [3]. Results for quantum mechanical DFT calculations [4] of low temperature plasmas will be presented. The dynamical structure factor and the response function for such finite nano plasmas are in the focus of interest. The relation between the bi-local correlation functions of the current and charge density will be presented, see [5]. Finally, these material properties allow to discuss the role of collective excitations and the damping of these excitations in nano plasmas.

- [1] C. Xia, C. Yin, and V.V. Kresin, Phys. Rev. Lett., 102, p. 156802, 2009.
- [2] T. Raitza, H. Reinholz, G. Röpke, I. Morozov, and E. Suraud, Contrib. Plasma Phys., 49, 498, 2009.
- [3] T. Raitza, H. Reinholz, I. Morozov, and G. Röpke, Phys. Rev. E, 48, 036406, 2011.
- [4] S.A. Chin and E. Krotscheck, Phys. Rev. E, 72, p. 036705, 2005.
- [5] T. Raitza, I. Broda, H. Reinholz, and G. Röpke, Contrib. Plasma Phys., 52, 118, 2012.



## Abstracts of posters: Session I Tuesday 11.09.2012, 17:30 - 19:30

- Statistical physics and *ab-initio* simulations Part 1
- Producing non-ideal plasmas (optical lasers, free electron lasers, heavy-ion beams, Z machine, high explosives etc.)
- Diagnostics of non-ideal plasmas (x-ray scattering, line shapes, stopping power, emission and absorption)
- Equilibrium properties, equation of state and phase transitions
- Dense astrophysical and inertial confinement fusion plasmas

Nr.	Name	Title of contribution
P I.1	A.B. Ashikbaeva	Static properties of Kelbg-pseudopotential-modelled plasmas
P I.2	A. Askaruly	Modelling of the dynamic conductivity of Kelbg-pseudopotential-modelled plasmas
P I.3	V.B. Bobrov	Virial theorem, one-particle density matrix, and equilibrium condition in an external field
P I.4	A.V. Chentsov	Isentropic Compression of Deuterium by Quantum Molecular Dynamics
P I.5	V.S. Filinov	Quantum simulation of thermodynamic and transport properties of quark–gluon plasma
P I.6	Zh.A. Moldabekov	Effective interaction potentials in two component semiclassical plasma
P I.7	T. Schoof	Configuration path integral Monte Carlo simulation of correlated fermions
P I.8	M.A. Voznesenskiy	Calculation of canonical properties of a quantum system by path integral numerical methods
P I.9	G. Zwicknagel	Classical-MD and wave-packet-MD simulations of nonideal plasma
P I.10	S. Bedacht	Cryogenic targets for experiments with laser and particle beams
P I.11	Q.F. Chen	Measurement of eqution of state for dense argon plasma under multi-shock compression to 150 GPa
P I.12	KJ. Chung	Evolution of plasma channel and shock wave in water spark discharge
P I.13	K. Falk	Measuring the equation of state of warm dense matter (WDM) aluminum
P I.14	M. Kelbg	Seeded multi-electron ionization of xenon doped helium droplets
P I.15	D. Nikolaev	Simultaneous measurements of pressure and temperature of lead vapor interaction with sapphire wall in ion-beam driven experi- ments
P I.16	N.A. Tahir	Generation of non-ideal plasmas at the HiRadMat facility at CERN using the Super Proton Synchrotron
P I.17	S.I. Tkachenko	Phase evolution of dense core during aluminum wire explosion
P I.18	Yu.B. Zaporoghets	The interaction of explosively driven dense plasma with a low intensity laser radiation
P I.19	A. Zarvin	On the possibility of intense clusters molecular beam formation
P I.20	R. Bredow	Hypernetted chain (HNC) calculations for the structure of dense multi-component plasmas
P I.21	B. Holst	Absorption of femtosecond laser pulses in gold foils at solid density
P I.22	K. Kimura	Inelastic X-ray Scattering Study of Plasmons in Solid and Liquid Rb
P I.23	D. Kraus	Melting of shock-compressed graphite characterized by X-ray scattering
P I.24	PM. Lang	The detector for the PRIOR proton microscope
P I.25	K. Lee	A finite element 1-D simulation of magneto-hydrodynamics for underwater electrical wire explosion
P I.26	N. Medvedev	Ultrafast electron kinetics in solid SiO <sub>2</sub> under X-ray
P I.27	KU. Plagemann	Calculation of the dynamic structure factor with ab initio simulations for warm dense matter
P I.28	M. Stransky	Optical emissions from Al target irradiated by FLASH with a self-similar model of plasma expansion
P I.29	R. Thiele	Hartree-Fock atom embedded in a charged environment
P I.30	S. Toleikis	Ultrafast non-equilibrium collective dynamics in warm dense hydrogen
P I.31	D. Varentsov	PRIOR - High energy proton microscopy at extremes

Nr.	Name	Title of contribution
P I.32	J. Vorberger	Applying X-ray Thomson Scattering to diagnose non-ideal Plas-
		mas
P I.33	NU. Bastian	Cluster virial expansion for partially ionized plasmas
P I.34	M.T. Gabdullin	Composition and thermodynamic properties of dense berrylium
		and carbon plasmas
P I.35	T. Ismagambetova	Thermodynamical properties of dense hydrogen plasma
P I.36	K.V. Khishchenko	Temperature and heat capacity of hydrocarbons in strong shock waves
P I.37	A.N. Kocharian	Spontaneous phase separation instabilities in finite two-dimensional Hubbard model
P I.38	Y. Omarbakiyeva	The second virial coefficient and scattering processes in partially ionized hydrogen plasma
P I.39	W. Schröer	The phase behavior of solutions of ionic liquids
P I.40	D. Semkat	BCS-type condensate in the electron-hole plasma of silicon
P I.41	A.A. Shadrin	Calculations of EOS and shock Hugoniots of metals using theoret-
		ical models of dense ionized matter
P I.42	A.S. Shumikhin	Free atoms metallization effect on shock-wave Hugoniot in hydro-
		gen and deuterium
P I.43	T. Sjostrom	Finite temperature Hartree-Fock and MD on confined hydrogen systems
P I.44	S. Trigger	Identity of electrons and ionization equilibrium
P I.45	E.V. Vasilieva	Polymorphic phase transitions in the system with the Yukawa and
		inverse-power potentials
P I.46	J. Vorberger	The equation of state of hydrogen in the physical picture
P I.47	S. Xiang	Equation of state model for metals in a wide region of pressure and temperature
P I.48	O. Zivny	Thermodynamics of high-temperature multicomponent thermal
		plasma
P I.49	A. Becker	Modeling Brown Dwarfs using an ab initio equation of state for
		hydrogen and helium
P I.50	M. Bethkenhagen	Equation of state and phase diagram of ammonia at high pressures
P I.51	D. Cebulla	Ab initio calculations for MgO at high pressures
P I.52	M. French	Ab initio simulations for material properties along the isentrope of Jupiter
P I.53	U. Kramm	Atmosphere and evolution of the young Hot Jupiter WASP-10b
P I.54	B.R. Lee	Electric fields and currents in thunderclouds
P I.55	CV. Meister	Application of the energy principle of ideal MHD to pinch plasmas
P I.56	R. Püstow	Saturn's cooling history considering the demixing of hydrogen and helium

## Statistical physics and ab-initio simulations – Part 1

### P I.1

## Static properties of Kelbg-pseudopotential-modelled plasmas

A.B. Ashikbaeva<sup>1</sup>, A. Askaruly<sup>1</sup>, D. Dubovtsev<sup>1</sup>

The partial radial distribution functions and static structure factors of hydrogen-like plasmas modelled with the Kelbg pseudopotential are calculated within the Ornstein-Zernike approximation. It is shown that the simulation data [1,2] on the inverse dielectric function satisfies five convergent sum rules and other exact relations. The sum rules which are the power frequency moments of the loss function are computed using the Kelbg potential. Thermodynamic characteristics of simulated systems are analyzed and conclusions with respect to the applicability of the Kelbg potential are drawn.

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### P I.2

## Modelling of the dynamic conductivity of Kelbg-pseudopotential-modelled plasmas

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The simulation data [1,2] on the dynamic collision frequency (DCF) of hydrogen-like plasmas modelled with the Kelbg pseudopotential are treated within the theory of moments with local constraints. Additionally, the correlational sum rule which is the second power frequency moment of the external conductivity real part is taken into account to express the DCF in terms of the Nevanlinna parameter function. The validity of the suggetsed analytic form of the latter is tested against the simulation data, while the sum rules are calculated using the Kelbg potential and the Ornstein-Zernike hypernetted-chain equations.

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#### P I.3

## Virial theorem, one-particle density matrix, and equilibrium condition in an external field

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Based on the analysis of the virial theorem and stress tensor, it is shown that the average energy of the Coulomb system under a static external field in a given volume is completely defined by a one-particle density matrix. In this case, one-particle density matrix satisfies the closed equation expressing the equilibrium condition in a given static external field. An expression for the pressure of a heterogeneous system of interacting particles is found.

### P I.4

## Isentropic Compression of Deuterium by Quantum Molecular Dynamics

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In this work we present our calculations of the compression isentrope of deuterium. For the calculations we use the plane-wave density functional code Vienna ab initio simulation package (VASP) [1] with the projector augmented wave pseudopotentials and generalized-gradient-approximation exchange-correlation functional. The quantum molecular dynamics approach which is based upon the Born-Oppenheimer approximation is applied to calculate pressure and internal energy of dense deuterium plasma.

The simulations were made for 64 atoms in a supercell with periodic boundary conditions. Initially the atoms were placed in a face-centered cubic crystal lattice, grouped by two atoms to form molecules. The temperature of the ions was controlled by a Nose thermostat, and was varied between 6500 K and 21000 K. The density of the system was fixed by the size of the supercell and was chosen in the range 0.9- $4.3 \text{ g/cm}^3$ . The system was equilibrated during 1000 steps in a lite regime (the plane-wave cut-off energy Ecut = 250 eV without pressure calculation) and during the next 1000 steps the thermodynamic parameters were averaged in the accurate regime (Ecut = 1200 eV).

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The time step of simulations was equal to 0.2 fs.

We used Zeldovich's approach [2] to restore the isentrope by solving a differential equation using thermodynamic properties, obtained from QMD simulations.

We reconstructed the compression isentrope of deuterium from the initial point with  $r_0 = 1.09 \text{ g/cm}^3$  and  $P_0 = 77 \text{ GPa}$ , this point corresponds to the lowest-pressure experimental point [3]. Also we obtained temperature data along the isentrope from the reconstruction.

The position of the calculated isentrope is smooth and shows no density jump registered experimentally [3, 4]. However, our temperature graph has a section with a flatter slope, just where the experimental isentrope shows a jump of density. Our estimations show that this fact is connected with rapid pressure ionization of deuterium in this part of the isentrope. This is also confirmed by the rise of electrical conductivity of deuterium in this area, calculated by means of the Kubo-Greenwood formula.

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### P I.5

## Quantum simulation of thermodynamic and transport properties of quark-gluon plasma

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For quantum simulation of thermodynamic and transport properties of quark-gluon plasma (QGP) within unified approach we combine path integral and Wigner (in phase space) formulations of quantum mechanics. Thermodynamic properties of a strongly coupled quark-gluon plasma (QGP) of constituent quasiparticles is studied by a color path-integral Monte-Carlo simulations (CPIMC). For simulations we have presented QGP partition function in the form of color path integral with new relativistic measure instead of Gaussian one used in Feynman and Wiener path integrals. For integration over color variable we have also developed procedure of sampling color variables according to the group SU(3) Haar measure. It is shown that this method is able to reproduce the available quantum lattice chromodynamics (QCD) data. The canonically averaged quantum operator time correlation functions and related kinetic coefficients are calculated according to the Kubo formulas. In this approach CPIMC is used not only for calculation thermodynamic functions but also to generate initial conditions (equilibrium spatial, momentum, spin, flavor and color quasiparticle configurations) for generation the color phase space trajectories being the solutions of related differential dynamic equations. Correlation functions and kinetic coefficients are calculated as averages of Weyl's symbols of dynamic operators along these trajectories. Using

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this approach we have calculated the diffusion coefficient and shear viscosity, which not bad agree with experimental data obtained at RIHC.

### P I.6

## Effective interaction potentials in two component semiclassical plasma

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In this work the effective screened pair potentials of charged particles interaction in the dense plasma, in which quantum effects are important, are presented [1]. These potentials were obtained on the basis of two methods. Firstly, the effective potential was calculated basing on the dielectric function obtained from MD data. MD simulation was performed on the basis of the interaction micropotential, which was obtained by the comparison of the quantum-mechanical Slater sum with the classical Boltzmann factor [2]. This micropotential correctly takes into account the diffraction effects in a wide region of the temperature [3]. Secondly, the effective potential was obtained on the basis of the same micropotential and the linear response theory in random phase approximation [4]. In both cases analytical expressions for effective pair interaction potentials were found. Analysis of behavior of these potentials in a wide region of plasma parameters was made. Results were compared with other knowing effective potentials of charged particles interaction.

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#### P I.7

## Configuration path integral Monte Carlo simulation of correlated fermions

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The configuration path integral Monte Carlo (CPIMC) approach for correlated many-particle systems with arbitrary pair interactions in a continuous space at finite temperatures is presented [1,2]. It is based on a representation of the N-particle density operator in a basis of (anti-)symmetrized N-particle states (configurations of occupation numbers). The method is applied to degenerate, correlated fermions in a two

dimensional trap. A Restricted Active Space approach is used to reach stronger couplings ( $\lambda \leq 4$ ) and larger particle numbers (N\leq 10). The efficiency of the method (fermion sign problem) is investigated and compared to standard direct fermionic path integral Monte Carlo and an exact diagonalization method.

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### P I.8

## Calculation of canonical properties of a quantum system by path integral numerical methods

Voznesenskiy M.A.<sup>1</sup>, Vorontsov-Velyaminov P.N.<sup>1</sup>

We propose a new approach in obtaining the partition function of a system of several interacting particles (fermions) in external field within path integral Monte Carlo method based on direct averaging of exchange contributions over the positive weight determined by non-closed trajectories. The complete partition function is then obtained at finite temperatures down to their low values. We found a good agreement of data obtained by the new method with results of previously proposed path-integral-expanded-ensemble Monte Carlo calculations [1,2]. The new approach allows us to reach observably lower temperatures thus permitting significantly to reduce the sign problem. The proposed approach yields an independent way to treat thermal properties of quantum systems, so the good agreement with previous data [1,2] allows us to test and state the validity of both approaches.

Simulations for systems of 2 up to 7 of non-interacting and interacting particles in harmonic or Coulomb field were performed. The presented approach allows one to carry out calculations for low temperatures that make it possible to extract data for the ground-state energy and low-temperature thermodynamics.

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## Classical-MD and wave-packet-MD simulations of nonideal plasma

G. Zwicknagel<sup>1</sup>

The dynamic properties of nonideal plasmas are studied by numerical simulations employing both wave packet molecular dynamics (WPMD) and standard classical molecular dynamics (MD) simulations. While in the WPMD method, which is based on a time-dependent variational principle, quantum effects are approximately taken into account by representing the electrons by localized Gaussian wave packets, the plasma is treated as a purely classical system in the standard MD, where essential quantum diffraction effects are modeled by regularizing the coulomb interaction at short distances.

Results of these numerical simulations of proton-electron plasmas are presented for the dynamic structure factor and the dynamic conductivity, and are compared to theoretical approaches like e.g. the RPA, DLFC and the Born-Mermin approximation (BMA). Special attention is paid to the comparison of the WPMD treatment and the MD simulations with effective potentials, in particular, concerning the role of the dynamics of the width of the wave-packets.

## Producing non-ideal plasmas

### P I.10

## Cryogenic targets for experiments with laser and particle beams

S. Bedacht<sup>1</sup>, G. Schaumann<sup>1</sup>, M. Roth<sup>1</sup>, D.H.H. Hoffmann<sup>1</sup>

In laser—plasma interaction experiments target geometry plays an important role. Micrometre thin cryogenic hydrogen targets could allow for achieving proton energies up to hundreds of MeV by exploiting new acceleration schemes different from Target Normal Sheath Acceleration (TNSA).

Besides ion acceleration, cryogenic targets are a viable tool for probing energy loss of heavy-ion beams in plasma.

In this poster, we present recent developments regarding the fabrication and characterization of ultra-thin cryogenic hydrogen targets.

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## Measurement of eqution of state for dense argon plasma under multi-shock compression to 150 GPa

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The plasma generated by an intense planar shock wave through dense gas and diagnostic configuration for the particle velocity profiles and time-resoved optical radiation histories were presented. With a dynamic technique of plasma generation and diagnostics in the pressure range of 2-150 GPa and temperature range of 20-30 kK for the equation of state of dense argon plasma were accurately measured by combining pyrometer and the Doppler pins system (DPS). The shock was produced using the flyer plate impact accelerated up to 6 km/s by a two-stage light gas gun and introduced into the plenum argon gas sample, which was pre-compressed from environmental pressure to about 20 MPa. The time-resolved optical radiation histories were acquired by using a muli-wavelength channel optical transience radiance pyrometer. Simultaneously, the particle velocity histories of the first-shocked sample impacts the optical window at the impact surface were measured with multi-DPS. The first shock wave velocity of sample was measured with the time-resolved histories and particle velocity was determined by the impedance-matching methods. The second shock pressure was derived from the measuring shock wave and particle velocity of window with pyromter and DPS, respectively. This technique is application to a wide variety of species and plasma conditions. The experimental data are compared with the calculated results from self-consistent fluid variational theory model in the partial ionization region.

### P I.12

## Evolution of plasma channel and shock wave in water spark discharge

Kyoung-Jae Chung<sup>1</sup>, Deok-Kyu Kim<sup>2</sup>, Kern Lee<sup>1</sup>, Seok-guen Lee<sup>1</sup>, Y. S. Hwang<sup>1</sup>

The temporal evolution of a plasma channel in water spark discharge and the propagation of shock wave into surrounding water are investigated. A set of one-dimensional time-dependent magnetohydrodynamic equations is solved in cylindrical coordinate with the equation of state for the high-temperature water plasma up to 50,000 K. The pressure and temperature of hot water plasma are obtained by solving the reaction equations with atomic and charge balance equations under the assumption of thermodynamic equilibrium. The electrical conductivity of hot water plasma at given temperature and density is calculated from the composition obtained from the reaction equations, in which both the electron-neutral collision and the electron-ion collision are considered. The temporal evolutions of the spark channel and shock front as well as

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the amplitude of the compressive wave are traced. Also, the numerical results are compared with some experimental observations.

### P I.13

## Measuring the equation of state of warm dense matter (WDM) aluminum

Katerina Falk<sup>1</sup>, John F. Benage<sup>1</sup>, David Montgomery<sup>1</sup>, James R. Williams<sup>1</sup>, Derek W. Schmidt<sup>1</sup>

We have carried out a set of experiments at the Omega laser facility to produce WDM aluminum at conditions near solid density and  $\sim 10$  eV with the goal of measuring the equation of state (EOS) of aluminum at those conditions. We are using a unique technique, the laser driven shock and release, to create our WDM target and facilitate the EOS measurements. This technique utilizes key new developments in HED experiments to enable measurements of pressure, density, and temperature. The new developments include recent shock results on low density aerogel foam that provide a well-characterized low density pressure standard and the development of a novel new imaging spectrometer to obtain x-ray Thomson scattering data, which is used to simultaneously determine the density, temperature and ionization state of WDM Al. The scattering measurement is complemented by velocity interferometry and optical pyrometry. We will present a description of the experimental technique along with pressure measurements and recent x-ray Thomson scattering results and their comparison with current theoretical EOS models.

### P I.14

## Seeded multi-electron ionization of xenon doped helium droplets

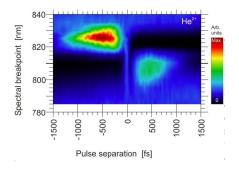
M. Kelbg<sup>1</sup>, N.X. Truong<sup>2</sup>, S. Göde<sup>1</sup>, J. Tiggesbäumker<sup>1</sup>, K.-H. Meiwes-Broer<sup>1</sup>

The impurity doping level dependence of the strong-field ionization of xenon-doped helium nanodroplets is studied using ultrashort tailored laser pulses. With the technique of colored double pulse fitness landscape (CDPFL)the dependencies on delay and energy distribution of the double pulse is systematically determined, see Fig. 2. As a result of the doping the transparent helium droplet turns into a strong absorber of femtosecond infrared pulses and is avalanche-like ionized in a two step process due to a delayed Mie plasmon resonanceabsorption of the second pulse. The influence of the Xenon-doping level on the laser-cluster resonance for the generation of highly charged Xe<sup>q+</sup>-Ions is discussed.

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CDPFL for He<sup>2+</sup> shows much higher yields for separated pulses under certain delay conditions. This behavior is strong evidence for a plasmon-resonant absorption induced by impurity.

# Simultaneous measurements of pressure and temperature of lead vapor interaction with sapphire wall in ion-beam driven experiments

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A result of experiments, performed at HHT area of GSI will be presented. An imaging displacement interferometer in a Twyman-Green configuration has been used to record a motion of a surface of sapphire window due to the impact of expanding target material (lead), heated by short ( $<100\mathrm{ns}$ ) pulse of uranium ion beam. Distance between sample and window were varied from 0.4 to 1.5 mm. Spatial and temporal velocity profiles allowed to calculate the pressure of a vapor layer near sapphire surface. Pressure distribution along the surface due to quasi-gaussian spatial profile of ion beam was clearly visible. Optical multichannel pyrometer was used to simultaneous recording of a lead surface and vapor temperature. The narrow-band dielectric mirror coating of a rear surface of sapphire window allowed to reflect the interferometer laser wavelength, remaining transparent to pyrometer bands. Pressures up to several kBars and temperatures more than 10 kK were recorded.

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## Generation of non-ideal plasmas at the HiRadMat facility at CERN using the Super Proton Synchrotron

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The Large Hadron Collider (LHC) is the most powerful particle accelerator in the world. Each LHC beam contains 362 MJ energy that is sufficient to melt 500 kg copper. Safety of operation is a very important issue when working with such awsome energies. Extensive numerical simulations have been done over the past decade to assess the damage caused by an accidental release of the beam energy at a single point [1,2]. It has been found that the range of the 7 TeV LHC protons is significantly extended due to the hydrodynamic tunneling effect. In order to check the validity of these simulations, a test facility named HiRadMat (High Radiation Material) has been constructed at CERN to carry out beam-target heating experiments using the 440 GeV proton beam generated by the Super Proton Synchrotron (SPS). Detailed numerical simulations have confirmed the existance of the hydrodynamic tunneling in case of the SPS beam as well. Experiments will be performed at the HiRadMat facility in the near future to check the validity of these simulations. This will also validate the simulations done for the case of the LHC beam.

A very interesting outcome of this theoretical work is that the target is severely damaged by the LHC as well as the SPS beam and a significant part of the target material is converted into High Energy Density (HED) state. It is therefore concluded that the HiRadMat facility can also be used to study HED physics.

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## Phase evolution of dense core during aluminum wire explosion

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In the numerical calculations it was obtained that, during the explosion of a single aluminum wire, the core material remains for a long time in the state of a dense nonideal plasma with a temperature of 1-3 eV. Only after shunting the main part of current to the corona, the core goes into a two-phase liquid-vapor state in the expansion process. However, if shunting of the current occurs at an early stage of the explosion, for example, when the wire material is still in liquid state, it is possible another scenario of core structure formation. In this case, due to a sharp drop of the compressive magnetic pressure, the core material can come into a state of the stretched melt during unloading. In accordance with the molecular dynamic calculations this metastable state decays, that resulting in to formation of a complex core structure: the outer cylindrical liquid shell filled with low-density foam. The foam decays into liquid droplets before the outer shell breaks apart. Simulated density profiles demonstrate good qualitative agreement with experimental high-resolution X-ray images showing the complex hollow structures within the long-living dense core.

### P I.18

## The interaction of explosively driven dense plasma with a low intensity laser radiation

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The investigation of explosively driven dense plasma using low intensity electromagnetic waves is an important diagnostic tool for studying transport properties of such medium. In particular, physical models describing the behaviour of matter under such conditions can be verified. However, to interpret correctly the results of reflectivity measurements it is necessary to know parameters of a transitive plasma layer. Angular dependence of s- and p-polarized reflectivities at several wavelengths can be used in the integration of corresponding Maxwell equations to construct the spatial profile of the density of charge carriers.

Here, the results of the new experiments on polarized reflectivities of explosively driven dense xenon plasma are presented. The study of polarized reflectivity properties of plasma was accomplished using laser light of wavelength  $\lambda = 694$  nm and  $\lambda = 532$  nm at incident angles up to  $\alpha = 0-70$ . With density up to  $r = 3.7g/cm^3$ , pressures r = 24

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GPa and temperatures up to  $T \sim 3 \cdot 10^4$  K of the investigated plasma, conditions with strong Coulomb interaction (the nonideality parameter up to  $\Gamma \sim 2.5$ ) were present. For determination of the equilibrium properties of explosively driven plasma, appropriate gas dynamics calculations were carried out. The plasma composition was calculated within a chemical picture. The integration of Maxwell equations are based on an interpolation formula for dc conductivity, obtained from a systematic quantum statistical treatment of different limiting cases. Results of the calculations with layer temperature profile and ea-collisions as factor are presented too.

To measure the dense xenon plasma polarized reflectivity coefficient, the pulsed Y3Al5O12:Nd3++KTP laser system with electro-optical shutter based on DKDP crystal and higher-order mode suppression of the laser radiation was used. For determination of the equilibrium properties of explosively driven plasma, appropriate gas dynamics calculations were carried out.

### P I.19

## On the possibility of intense clusters molecular beam formation

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Today beams of atomic or molecular ions are in fact become an integral part of many modern technologies (Giannuzzi and Stevens, 2004, Orloff, 2008). Conventional now ion cleaning, etching, implantation, sputtering and deposition of thin films of various materials - all of which are based essentially on the individual collisions (or a cascade of binary collisions) of incident ions with near-surface atoms.

A completely different situation occurs during a collision the energetic large clusters with the surface. In this case, nearly simultaneous interaction of many particles of cluster around the same number of atoms in a solid occurs. This leads to deposition a high-energy density into a very small volume of the target material, and strong nonlinear effects: lateral sputtering, dry etching, and shallow implantation. Recently it was shown that the accelerated gas cluster ion beams have a number of unique advantages that allow them to be considered a promising basis for new technologies, including nanotechnologies (Popok and Campbell, 2006, Yamada, 2007).

The work was performed on an experimental setup LEMPUS of Novosibirsk State University. A detailed description of the installation was given earlier. In this paper the possibility of accelerating gaseous cluster-ion beams for nanomaterials processing are discussed. In order to realize surface processing technology, a high-energy gas cluster ion beam irradiation system was developed. The results of the experimental study of formation of an intense cluster-ion beam of argon and mixtures are presented. The fundamental phenomenon influences on the main parameters of cluster-ion beam are considered. As a result of experimental investigations the optimal conditions for the formation of a clustering molecular beam from supersonic jets of argon have been determined. A maximum intensity of  $4 \cdot 10^{14}$  clusters/cm<sup>2</sup>\*sec for the clusters with an average size of 1000 molecules, and  $8 \cdot 10^{13}$  for clusters with an average size of more than 20,000 molecules have been reached. The possibility of increasing the intensity of the cluster molecular beam with small additions of easily condensable impurities was considered.

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## Diagnostics of non-ideal plasmas

### P I.20

## Hypernetted chain (HNC) calculations for the structure of dense multi-component plasmas

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Integral equation methods are used to study the structural properties of dense multicomponent plasmas. Information on the structural properties, e.g., the structure factors, can be used for the interpretation of Thomson scattering experiments at Free Electron Laser Facilities such as FLASH, LCLS or the future XFEL in Hamburg. We solve the Ornstein-Zernicke equation within the hypernetted chain (HNC) equation using effective pair potentials. The influence of different effective pair potentials as the Kelbg potential or the Deutsch potential will be discussed. The latter includes also electron exchange effects in zeroth order. An important extension is the description of non-equilibrium plasmas. Often, plasmas interacting with lasers can be described as two-temperature systems where the electrons have a temperature considerably higher than that of the ions. We will give the derivation of Ornstein-Zernicke equations for such multi-temperature systems basing on a generalized statistical operator. We propose a new ansatz for the effective temperature which has to be attributed to the electron-ion interaction. Results will be presented for pair distributions functions and static structure factors for dense hydrogen, beryllium, carbon and CH plasmas.

#### P I.21

## Absorption of femtosecond laser pulses in gold foils at solid density

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A model for the temporal evolution of a thin gold foil after being irradiated by a femtosecond laser pulse is presented. Ultrashort laser pulses excite electrons, which thermalize to very high temperatures within a few femtoseconds. In contrast, the ionic lattice is unaffected on the time scale of the laser pulse. The energy transfer from the hot electrons to the ionic degrees of freedom is a slower process. A new equilibrium temperature is not reached before several picoseconds have passed. This

non-equilibrium system can be described using the two-temperature model, which is a composition of two subsystems: one consisting of hot electrons and the other of an ionic lattice at low temperature. We studied the dynamics of the heating process and its effects on the optical properties of gold. Density Functional Theory enabled us to compute the dielectric function and material parameters, like heat capacities, which are used as input for the two-temperature model. We additionally used ab initio linear response to compute the phonon spectrum and the electron-phonon coupling constant within Density Functional Theory for several electronic temperatures of few eV.

#### P I.22

## Inelastic X-ray Scattering Study of Plasmons in Solid and Liquid Rb

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Conduction electrons in metal can be regarded as a typical example of degenerate plasma. The collective motion of conduction electrons is called plasma oscillation (plasmon). Plasmons give us valuable information on the properties of degenerate plasma, especially on the interactions between constituent electrons.

Plasmon behaviors of alkali metals in the solid state were previously investigated by vom Felde et. al. with electron energy loss spectroscopy (EELS) [1]. The EELS experiment revealed that the plasmon dispersions in heavy alkali metals, Rb and Cs, seriously deviate from the predictions of many-particle theories [2, 3] based on the interacting electron gas model. In order to solve this problem, Aryasetiawan and Karlson carried out the ab initio calculations [4], suggesting that plasmon dispersions in heavy alkali metals are strongly influenced by the interband transitions to the empty d state (band structure effect).

In the present study, we carried out the inelastic x-ray scattering measurements to determine the plasmon dispersions in solid (room temperature) and liquid (333 K) Rb in the range of momentum transfer 0.18 < q < 0.90 /Å. The measurements were performed on the Taiwan inelastic x-ray scattering beam line BL12XU at SPring-8. We observed higher plasmon excitation energies in the liquid state than in the solid state for large q, which can be interpreted as the reduction of the band structure effect. We also determined the q dependence of the line width and found smaller line width in the liquid state than in the solid state for small q, which might reflects the vanishing of Umklapp process on melting. The observed features of the plasmon excitation energy and line width suggest that metallic liquid is a more appropriate system than crystalline solid in terms of understanding the interactions between electrons in degenerate plasma.

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## Melting of shock-compressed graphite characterized by X-ray scattering

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We present measurements of the melting of graphite in a laser-driven shock experiment applying X-ray scattering. Laser radiation with intensities of  $\sim 2 \cdot 10^{13} \ \mathrm{W/cm^2}$  compressed the carbon samples by a factor of two reaching pressures of  $\sim \! 130 \ \mathrm{GPa}$ . Due to disintegration of the crystalline structure, the scattered signals of the probe radiation were modified significantly in intensity and spectral composition compared to the scattering on cold samples. The presence of the liquid state could clearly be identified by analysing scattering signals from two different scattering angles. Comparing the elastic and inelastic scattering features, structure factors could be obtained. These are compared to theoretical calculations from ab-initio simulations in this presentation.

### P I.24

## The detector for the PRIOR proton microscope

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While the idea to use charged particles for radiography is known since 1960's, the technique was not widely used because scattering in the radiographed sample caused a substantial image blur. A way to overcome this blur was discovered in the 90's at the Los Alamos National Laboratory by using a set of magnetic quadrupole lenses to image the object on the detector, and to correct chromatic aberrations.

Based on this experience, the proton microscope PRIOR (Proton Microscope for FAIR) is currently under construction at GSI. Its spatial resolution of less than 10  $\mu$ m will by far exceed the capabilities of other proton radiography systems available at LANL (Los Alamos) and ITEP (Moscow).

Here we present a first design of the designated detector system for future dynamic experiments with PRIOR, which consists of a scintillator screen and a high resolution CCD camera.

Geant4 Monte Carlo simulations have been carried out for optimizing the detector performance.

## A finite element 1-D simulation of magneto-hydrodynamics for underwater electrical wire explosion

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A one-dimensional (1-D) magneto-hydrodynamic (MHD) simulation code was developed for investigating the physics of non-ideal plasma generated in Underwater Electrical Wire Explosion (UEWE) experiments. The MHD code was written in Lagrangian description with discontinuous Galerkin finite element method (DG-FEM), which has definite advantages to handle the transient system in complicated geometry. Thus, it is applicable to describe fast transient MHD problem under extreme conditions such as fast expansion of non-ideal plasma channel in the water with ease. Our 1-D code, as a preliminary part of the development of 2-D simulation code, evaluated suitability of its own structure i.e., DG-FEM and Lagrangian description. Also the performance of code is verified by comparing to the results using finite volume based 1-D Lagrangian MHD simulation code [1]. The same equation of state and electrical conductivity models of metal plasma are applied to both simulations based on the reference paper. Some issues related to numerical treatment will be also discussed.

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### P I.26

## Ultrafast electron kinetics in solid SiO<sub>2</sub> under X-ray

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When a dielectric is irradiated with an ultrashort laser pulse at X-ray photon energy, various physical processes take place. The photons are absorbed mostly by the deep-shell electrons, which are then excited to the high energy states of the conduction band and/or to the continuum. These electron propagate further and perform secondary scatterings via elastic and inelastic channels. All these processes occur on femtosecond timescales. Material properties are then defined by the transient state of the electronic distribution within the solid. In this contribution we present a theoretical study of the ultrafast electron kinetics in solid  $SiO_2$ , irradiated with the femtosecond X-ray laser pulse ( $\sim$ 40 fs duration). The Monte-Carlo code, similar to [1,2] is applied

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to model the electron kinetics, which includes the primary ionization, secondary scattering of electrons, and Auger-decays of deep-shell holes. With the calculated transient electron density, the change of the optical properties (reflection, transmittance) of the material is estimated. The analysis of the results allows us to conclude that in the X-ray excited dielectric, the holes in the valence band give the dominant contribution to the the optical properties of the material.

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### P I.27

## Calculation of the dynamic structure factor with ab initio simulations for warm dense matter

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Warm dense matter of solid-like densities and temperatures of several eV is relevant for planetary interiors and inertial confinement fusion experiments. A versatile and reliable tool to probe such extreme states of matter is X-ray Thomson scattering (XRTS) which gains information about plasma parameters like electron density, electron temperature and mean ionization state directly from the dynamic structure factor [1]. Such XRTS experiments have already been performed on beryllium for different conditions [2, 3]. We calculate the dynamic structure factor in warm dense beryllium by means of ab initio molecular dynamics simulations. The dynamic conductivity is derived from the Kubo-Greenwood formula [4], and a Drude-like behaviour is observed. The corresponding dielectric function is used to determine the dynamic structure factor. Since the ab initio approach is so far only applicable for wavenumbers  $\mathbf{k}=0$ , the k-dependence of the dielectric function is modelled via the Mermin ansatz. We present results for the dielectric function and the dynamic structure factor for beryllium and compare with perturbative treatments such as the Born-Mermin approximation.

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## Optical emissions from Al target irradiated by FLASH with a self-similar model of plasma expansion

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This report touches experiments in which the soft x-ray laser beams (13.5 nm) from FLASH were focused on aluminum targets as reported in the papers "XUV Spectroscopic Characterization of Warm Dense Aluminum Plasmas generated by the Free-Electron-Laser FLASH" by U. Zastrau et al., and "Optical emission spectroscopy of various materials irradiated by soft x-ray free-electron laser" by J. Cihelka et al. The later one noticed the absence of aluminum ion lines in the near-optical and the optical range (200-600 nm), which is the subject of the present contribution. The adiabatic expansion of aluminum plasma into vacuum with recombination processes was modeled using a self-similar solution. Preliminary results show that in the case of lower laser intensities ( $10^{13} \text{ W/cm}^2$ ) the plasma is cooled by the expansion in such a way that at the time when it becomes transparent in the optical range, it has low enough temperature to emit the atomic lines only. In the case of a tighter focus ( $I \sim 10^{16} \text{ W/cm}^2$ ), a higher plasma temperature during the expansion supports some small traces of ion lines.

### P I.29

## Hartree-Fock atom embedded in a charged environment

Robert Thiele<sup>1</sup>

The new X-ray free electron lasers (XFELs) are a promising tool for structural determination of macromolecules and biomolecules, using coherent diffractive imaging. During imaging the intense XFEL pulses also ionize the molecule efficiently, creating core-hole states within deep atomic shells. The photoinduced processes such as X-ray absorption, subsequent Auger decay or fluorescence emission have to be analyzed in detail. In particular, it is important to estimate how the charged environment within the molecule modifies the ionization thresholds and rates for these processes, comparing to the case of an isolated atom. Here, we apply the XATOM toolkit to obtain predictions on the modified ionization thresholds and rates of some photoinduced processes in carbon. The Hartree-Fock-Slater model is extended so as to include the electron screening and ion correlation effects, induced by the charged environment of an atom/ion. For electron screening two models, Debye model and ion-sphere model, corresponding to weakly and strongly coupled electron plasma regimes, are considered. Ion correlations are treated with radial distribution function, estimated for liquid carbon. With these approaches we obtain predictions on modifications of orbital energies, photoabsorption cross sections, Auger decay and fluorescence emission rates, induced by the charged environment of an carbon atom/ion, as a function of charge density and temperature. We find significant modifications, when compared to the case of an isolated atom.

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Our results have implications for studies of evolution of XFEL irradiated samples, in particular for those dedicated to the coherent diffraction imaging.

#### P I.30

## Ultrafast non-equilibrium collective dynamics in warm dense hydrogen

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We present collective Thomson Scattering with soft x-ray Free Electron Laser radiation as a method to track the evolution of highly transient warm dense plasmas with 100 fs time resolution. In a pump-probe scheme, a fs 800 nm laser heats liquid hydrogen droplet of different size. With a variable time delay, 13.5 nm light probes this plasma state and the scattered soft x-ray spectra are recorded for different scattering angles. The total scattered intensity shows a special dynamic behavior as function of time, directly linked with the electron – ion energy relaxation. The scattering angle behavior reveals an inhomogenously heated sample. Free electron temperature and density can be inferred from plasmon shifts and the plasmon intensity ratio, ultimately gaining information about the warm dense matter equation of state. Without optical pump, the interaction of soft x-ray light with the target has been measured as self Thomson Scattering. In particular, the electron-electron equilibration time scale has been investigated [1,2].

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## PRIOR - High energy proton microscopy at extremes

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High energy proton microscopy (HEPM) provides unique capabilities in penetrating radiography including the combination of high spatial resolution and field-of-view, dynamic range of density for measurements, in addition to the key attribute of reconstructing the density variations to less than 1% inside volumes and in situ environments. The PRIOR (Proton Microscope for FAIR) facility which is currently being constructed at GSI will use a 4.5 GeV proton beam from the SIS-18 synchrotron and allow for a significant step forward in spatial resolution (> 10  $\mu$ m) to advance high-energy-density physics and heterogeneous materials research. In this paper we discuss the status of the PRIOR project and proposed HEPM experiments in different fields from non-ideal plasma physics to particle radiosurgery.

#### P I.32

## Applying X-ray Thomson Scattering to diagnose non-ideal Plasmas

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Driven by the impressive progress in experimental capabilities, research on matter with high energy density has dramatically changed over the last decade. The availability of high-energy lasers facilities, such as the National Ignition Facility in Livermore and the Omega Laser Facilities in Rochester, USA, makes it nowadays possible to create and investigate matter under extreme conditions that naturally only occur in astrophysical objects. Of particular interest are hereby states of warm dense matter (WDM) which are highly non-ideal systems characterised by strong forces between the ions and partial degeneracy within the electron component. The complex nature of WDM poses great challenges in the theoretical description as standard expansion techniques known from plasma or solid state theories lose their applicability.

Recently, X-ray Thomson scattering has become an indispensable diagnostic tool for high-energy density matter. However, this method significantly relies on well-founded theoretical models for the dynamic electron and ion structure of this highly non-ideal state and is currently limited to matter consisting of single components or in simple conditions. In this contribution, we will demonstrate how the theoretical framework has to be extended to describe systems containing multiple chemical elements or different ionisation stages. Thereby, the approach takes all mutual correlation between the various species and the electrons fully into account allowing to go beyond the linear response approximation. We will describe the extraction process of basic plasma parameters from the scattering signal highlighting the adjustments due to the occurrence of another ion species in a multi-component material. These improvements will

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enhance the capability of x-ray Thomson scattering as reliable diagnostic tool to investigate non-ideal systems with an arbitrary number of ion species as it occurs in nature, technical applications and WDM experiments.

## Equilibrium properties, equation of state and phase transitions

#### P I.33

### Cluster virial expansion for partially ionized plasmas

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The chemical picture serves as an intuitive concept to treat the low-density limit of many-particle systems forming clusters (bound states). Systematic quantum statistical approaches allow to combine the mass action law with mean-field concepts.

Within a generalized Beth-Uhlenbeck approach, the quasiparticle virial expansion and the suppression of correlations due to screening and Pauli blocking is formulated.

This approach is generalized to include arbitrary clusters, where special attention must be paid to avoid inconsistencies such as double counting. The contribution of the continuum to the virial coefficients can be reduced considering separately excited states and quasiparticle energies.

The cluster-virial expansion connects known benchmarks at low densities as well as at high densities. In detail the electron, proton and atom system is considered.

#### P I.34

## Composition and thermodynamic properties of dense berylium and carbon plasmas

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In this work composition and thermodynamic properties (chemical potentials, internal and free energy, equation of state) of dense beryllium and carbon plasmas were investigated. Partially ionized plasma is a multi-component system that contains electrons, ions, and atoms. The interaction between particles causes decreasing of the ionization potential compared with isolated atoms and ions. The effective potential was used for describing the electron-electron and electron-ion interactions. This effective potential takes into account the effects as charge screening at long distances and short range quantum mechanical effects of diffraction and symmetry. These effects occur in dense

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systems. A similar effective potential has been used for describing of ion-ion interaction. The charge-atomic interaction was described by effective polarization potential, which also takes into account the screening effects and quantum effects of diffraction. The excess of chemical potential was calculated within the effective potential models. Obtained results were used for investigation of composition of dense beryllium and carbon plasmas by numerical solving the system of the Saha equations with corrections to nonideality (lowering of ionization potentials). The results are compared with results of other authors.

#### P I.35

## Thermodynamical properties of dense hydrogen plasma

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This paper considers a dense hydrogen plasma consisting of electrons and ions. Various approaches are used for description of plasma properties with different parameters. At the calculation thermodynamic functions of a nonideal plasma difficulties related to interaction of particles are haven. There are also especial difficulties at investigations of partially ionized plasma properties since it is necessary to know the interaction potentials. Such potentials should take into account the specific effects existing in the considered area of densities and temperatures. For calculations of thermodynamic characteristics (internal and free energy and equation of state) effective potentials for electron-electron and electron-ion interactions [1] were used taking into account screening effect at large distances and quantum-mechanical effects of diffraction and symmetry [2] at small distances. The effective potential for ion-ion interaction was chosen in work [3]. Excess parts of the thermodynamic functions of a nonideal system have been derived from the radial distribution functions of particles in this system. The obtained results were compared with the data of other authors.

#### P I.36

## Temperature and heat capacity of hydrocarbons in strong shock waves

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Equations of state for different materials over a wide range of thermodynamic parameters are necessary for numerical simulations of physical processes in plasmas at high energy densities. Reliability of the calculation results is determined mainly by adequacy of description of medium properties. In the present work, a thermodynamic model of free-energy potential is presented for hydrocarbon compounds. On the basis of

this model, equation-of-state calculations are carried out for polyethylene, polypropylene and polystyrene at high pressures and temperatures. Obtained results are in a good agreement with available data from experiments with strong shock waves.

### P I.37

## Spontaneous phase separation instabilities in finite two-dimensional Hubbard model

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Spontaneous phase separation instabilities with the formation of various types of charge and spin pairing (pseudo)gaps in U>0 Hubbard model including the next nearest neighbor coupling are calculated with the emphasis on the two-dimensional (square) lattices generated by 8- and 10-site Betts unit cells. The exact theory yields insights into the nature of quantum critical points, continuous transitions, dramatic phase separation instabilities and electron condensation in spatially inhomogeneous systems. The picture of coupled antiparallel (singlet) spins and paired charged holes suggests full Bose condensation and coherent pairing in real space at zero temperature of electrons complied with the Bose-Einstein statistics. Separate pairing of charge and spin degrees at distinct condensation temperatures offers a new route to superconductivity different from the BCS scenario. The conditions for spin liquid behavior coexisting with unsaturated and saturated Nagaoka ferromagnetism due to spin-charge separation are established. The phase separation critical points and classical criticalities found at zero and finite temperatures resemble a number of inhomogeneous, coherent and incoherent nanoscale phases seen near optimally doped high-Tc cuprates, pnictides and CMR nanomaterials.

### P I.38

## The second virial coefficient and scattering processes in partially ionized hydrogen plasma

Yultuz Omarbakiyeva<sup>1</sup>, Gerd Röpke<sup>2</sup>

In the plasma physics, the investigations on equation of state constitute the area of greatest concern. This can be justified by an attempt to describe adequately the plasma state and processes at a large range of temperature and number density. In this paper we study equation of state using the quantum statistical methods. We consider the cluster-virial expansion for a partially ionized hydrogen plasma, which consists of not only electrons, ions and atoms but also heavier clusters, such as molecules or molecular ions. The exact quantum mechanical expression for the second virial coefficient was given by Beth and Uhlenbeck [1]. They showed that the second virial coefficient can be expressed in terms of scattering phase shifts and bound state energies.

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Calculation of the second virial coefficient by Beth-Uhlenbeck formula gives a possibility to observe the formation or disappearance of the bound states and its influence on the thermodynamics of the system. The second virial coefficients for the charged components e-e, e-i and i-i was already considered in Refs.[2, 3], but the coefficients for bound states still present large interest. For the e-H pairs, the second virial coefficient was calculated using experimental and theoretical values for the phase shifts in the singlett and triplett channel [4]. A separable potential was constructed to reproduce these phase shifts. Within a generalized Beth-Uhlenbeck approach, density effects such as Pauli blocking have been incorporated. This approach can be extended to include further components of the plasma, in particular the formation of H<sub>2</sub> molecules. Using experimental data of the scattering phase shifts of e-H<sub>2</sub> one can discuss the consequences for the equation of state, and give corresponding coefficients of cluster virial expansion.

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### P I.39

## The phase behavior of solutions of ionic liquids

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The knowledge of thermodynamic properties like phase-diagrams of Ionic Liquids (ILs) is a prerequisite for application in chemical engineering. A large number of studies dealing with the physico-chemical characterization of IL systems can be found in the literature, but systematic studies focusing on the phase behavior are still rare.

To this end we have studied the liquid-liquid (LLE) phase behavior of mixtures of different ILs with alcohols and non-polar hydrocarbons. Applying the cloud point method the LLEs were determined in a temperature range of  $275-423~\mathrm{K}$  at ambient pressure. Partial miscibility with upper critical solution temperatures (UCST) is usually observed increasing with the chain lengths of the alcohols and decreasing with the length of the side chain of the cation. In water and diols, however, the UCSTs increase with the length of the alkyl-chains of the ILS.

A numerical analysis of the phase diagrams is consistent with Ising criticality. Concepts for the description of the asymmetry of the phase diagram presuming the validity of the rectilinear diameter rule or a non-linear diameter requested by the theory of complete scaling are applied.

The systematic trends of the phase behavior and the results of the analysis (UCST, critical composition, width and diameter of the phase diagrams) are discussed in detail. Comparison with the predictions of the model systems of charged hard spheres is made. The application of corresponding phase behavior on the systems investigated

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so far yields one single master-curve. Furthermore simple empirical relationships are formulated, that allow for the description or estimate of UCSTs of the IL-alcohol family. A mean-field lattice model is proposed that enables rationalizing the observed regularities between size and shape of the ILs and the solvents.

### P I.40

## BCS-type condensate in the electron-hole plasma of silicon

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Quantum condensation phenomena in highly excited semiconductors comprise, besides the Bose-Einstein condensate of excitons, also a BCS-type condensate of weakly correlated electron-hole pairs at very low temperatures and high densities, where excitons can no longer exist.

The key quantity of the BCS condensate is the so-called gap function. We present theoretical results for this quantity based on a recent approach [1]. The gap function modifies the single-particle spectrum of the carriers. These modifications are transformed in the usual way [2] into alterations of the high-energy tail of the electron-hole pair luminescence spectrum. Therefore, the occurrence of BCS condensed electron-hole pairs, i.e., a nonzero gap function, should manifest itself in the luminescence spectrum.

We present first experiments where the electron-hole plasma in silicon is captured in a stress-induced potential trap at temperatures below 100 mK. Results for the measured spectra are shown and compared to the theoretical predictions.

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### P I.41

### Calculations of EOS and shock Hugoniots of metals using theoretical models of dense ionized matter

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Study of thermodynamic and optical properties of dense nonideal plasma is the one of the actual concepts of fundamental research of matter in extreme conditions. It's important for the solution of wide range of high energy density physics (HEDP) applications: to simulate the interaction of laser pulses with matter, different astrophysical applications and many other important tasks. Therefore the development of realistic

physical models and calculations methods to solve these tasks are of great importance. We present the results of calculations of equations of state (EOS) and shock Hugoniots of metals with shell effects accounting using quantum-statistical cell model of Liberman [1,2] and so called chemical model (CP) of dense plasma [3-6] using superconfiguration (SC) approach [7] (CP-SC) that implemented in the RESEOS code and EOSC code. Calculations were done in wide range of densities and temperatures that are important for different HEDP applications. Calculated shock Hugoniots and thermodynamic functions are compared with data calculated using Thomas-Fermi model [8,9] and Klinishov' EOS [10] widely used in practical calculations. Importance of shell oscillation for EOS calculations also discussed.

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#### P I.42

# Free atoms metallization effect on shock-wave Hugoniot in hydrogen and deuterium

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The dissociation phenomenon in the shock wave compression of molecular liquids (H2, D2, N2, O2, CO) was detected in experiments at high pressure (30-150 GPa) and rather low temperatures (5-8 kK). The usual mechanism of thermal dissociation is not applicable to describe the phenomenon of observable dissociation because of temperatures are low in comparison with dissociation energies of molecules (5-7 eV). We have supposed that interaction between free atoms in a dissociating atomic-molecular mixture is caused by the collective quantum cohesive energy, that analogous the binding energy of atoms in alkali metals. We can speak about metallization of free atoms [1]. The Wigner-Seitz approximation is used for cohesive energy calculation. We have obtained approximate solution of Schrödinger equation for ground state of quasi-atomic liquid. The derivation of wave function on the bound of the Wigner-Seitz cell is equivalent to

zero. The received energy of the ground state decreases under compression (increases in absolute value) in comparison with energy of the ground state of hydrogen atom. Obtained energy is agreed with available numerical calculations. The atom radius also decreases. The cohesive energy is sum of the ground state energy and the Fermi kinetic energy of the delocalized electrons. The fraction of these electrons is proportional to a square of a wave function of the ground state on a cell bound [2]. The presence of the collective cohesive energy between the free atoms with a minimum allows to speak about possibility of quasi-liquid behavior of the atomic component in the dissociated atomic-molecular mixture. Our calculations have shown, that within the frameworks of our hypothesis the transition to the dissociated state has the character of the firstorder phase transition - the transition from the molecular fluid in a atomic liquid with critical temperature  $\sim 10 \text{ kK}$  and density jump for hydrogen (0.7-1) g/cm<sup>3</sup> at temperature 4 kK. We investigate the free atoms metallization effect on Shock-Wave Hugoniot in Hydrogen and Deuterium. The region of ambiguity on Shock-Wave Hugoniot is discovered. Shock-Wave Hugoniot have discontinuity. The Master equation for Hugoniot adiabat have one ore three roots. This region is close to experimentally fixed region of ambiguity for Shock-Wave Hugoniot in Hydrogen and Deuterium [3, 4].

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### P I.43

# Finite temperature Hartree-Fock and MD on confined hydrogen systems

Travis Sjostrom<sup>1</sup>

Warm dense matter (WDM) systems at significant temperatures (e.g.,  $T \sim 1$  – several eV) and densities (e.g. one or more orders of magnitude more dense than solid) are of increasing interest but challenging. So far, detailed studies of WDM generally use Born-Oppenheimer molecular dynamics (BOMD) with ground-state density functional theory (DFT) approximations. To understand the implications of this approach as well as provide insight for development of orbital-free free energy density functionals, we have developed and implemented the thermal Hartree-Fock (tHF) approximation for ions confined in hard-walled box. Though HF schemes have known limitations, the strategic advantage of this approach is that it utilizes a completely well-defined model. Initial studies with a small number of ions at fixed positions already have been published [1]. Here we report progress regarding arbitrary ionic positions. First we consider static arrays with both low and high symmetry relative to the box geometry. Then we report first results on tHF-BOMD. In addition, we compare some of the static tHF results directly with approximate density functional results, including those from finite-temperature orbital-free kinetic and exchange functionals.

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A finite temperature version of second order perturbation theory (MP2) is considered to compare with finite temperature correlation functionals.

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### P I.44

## Identity of electrons and ionization equilibrium

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It is perhaps appropriate that, in two years later the 90th anniversary of Meghnad Saha seminal paper (1920), new developments should call fresh attention to the problem of ionization equilibrium in gases. Ionization equilibrium is considered in the simplest "physical" model for an electronic subsystem of matter in a rarefied state, consisting of one localized electronic state in each nucleus and delocalized electronic states considered as free ones. It is shown that, despite the qualitative agreement, there is a significant quantitative difference from the results of applying the Saha formula to the degree of ionization. This is caused by the fact that the Saha formula corresponds to the "chemical" model of matter.

### P I.45

# Polymorphic phase transitions in the system with the Yukawa and inverse-power potentials

Vasilieva E.V.<sup>1</sup>, Vaulina O.S.<sup>1</sup> <sup>1</sup>JIHT RAS

Here we present a simple analytical approach for calculation of phase diagram for polymorphic fcc-bcc transition (transition from a face-centered-cubic (fcc) crystal to a body-centered-cubic (bcc) solid) in the systems of particles interacting with potentials of Yukawa type and with inverse-power-potentials. These models (in various combinations) are commonly used for simulation of repulsion in physical kinetics of interacting particles (for example, in plasma physics, medicine, biology, physics of polymers, etc.). We present a new analytical criterion for determination of lines of fcc-bcc polymorph transition in the systems with isotropic repulsive potentials. This criterion has been obtained using the assumption of a minimum of potential energy in a steady phase and the condition of formation of configuration phase transition. A comparison of proposed approach with existing numerical and theoretical data is presented for Yukawa systems and the systems with inverse-power potentials; we can see a good agreement between our results and existing numerical data. Influence of a non-linearity of pair interaction forces on the structural phase transitions curves has been considered. Finally we have

to note that the scope of proposed approach is not limited by considered potentials. The proposed model may be easily adapted for a wide range of systems with isotropic repulsive potentials.

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### P I.46

## The equation of state of hydrogen in the physical picture

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Modern first principle numerical simulations like density functional molecular dynamic or quantum Monte Carlo have changed the approach to equation of state calculations. It now seems possible to calculate the equation of state over the entire phase space without need to revert to methods in the chemical picture. We show how density functional molecular dynamics simulations agree with fugacity expansion EOS in the low density limit and with two-fluid type approaches in the high density limit. We also revisit the two fluid model and show a new approach to two fluid models based on the Green's function approach. This method uses the charging formula to incorporate strong correlations. In order to do so, we try to take advantage of recent advances in the calculation of local field corrections.

#### P I.47

# Equation of state model for metals in a wide region of pressure and temperature

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Usually accurate equation of state (EOS) can only be used in a narrow region of pressure and temperature (PT). EOS model like QEOS can be employed to describe hot dense matter but not so accurate for the "cold" dense matter. We propose an EOS model. In this the Helmholtz free energy F per ion can be separated as static zero temperature energy, the electronic contribution and the vibrational contribution. The static zero temperature energy can be represented by Vinet-based model. For solid and liquid the, static zero temperature energy can be calculated in the framework of Mermin theorem. For plasma, this part are fitted to Thomas-Fermi model. The vibrational contribution for all phases can be expressed using a particle-in-cell based model. Based on this EOS model, EOS of metal Pt in a wide range are given.

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### P I.48

# Thermodynamics of high-temperature multicomponent thermal plasma

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The simple method for the calculation of the composition and thermodynamic properties of high-temperature multicomponent thermal plasma is presented. This approach proposed allows to avoid atomic electronic partition function divergency problem in thermodynamically consistent way, which is formulated in combination with the non-stoichiometric algorithm for the free energy minimization of the system. The proposed computational protocol makes it possible to include also intermolecular interactions.

## <u>Dense astrophysical and</u> inertial confinement fusion plasmas

### P I.49

## Modeling Brown Dwarfs using an ab initio equation of state for hydrogen and helium

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Models of the interior of Giant Planets and Brown Dwarfs rely on the equation of state (EOS) data for hydrogen, helium and water, as a representative of all heavier elements, which have usually considerable uncertainties in the high-pressure domain. We constructed a wide-range EOS for hydrogen and helium. The hydrogen EOS consists of data given by Leachman [1] and derived from fluid variational theory [2] for the low-density range ( $\rho < 0.2 \text{ g/cm}^3$ ). EOS data derived from finite-temperature density functional theory molecular dynamics (FT-DFT-MD) [3] have been used for intermediate densities ( $0.2 \text{ g/cm}^3 < \rho < 70 \text{ g/cm}^3$ ), and the Chabrier-Potekhin model was considered for high densities ( $\rho > 70 \text{ g/cm}^3$ ) [4]. The helium EOS consists of ideal plasma data for  $\rho < 0.1 \text{ g/cm}^3$ , FT-DFT-MD data for  $0.1 \text{ g/cm}^3 < \rho < 100 \text{ g/cm}^3$ , and the Chabrier-Potekhin model [4] for  $\rho > 100 \text{ g/cm}^3$ . Using this wide-range EOS data we model Brown Dwarfs in a fully convective one-layer model. We derive interior structure profiles and mass-radius relationships and compare our results with those derived using the Saumon-Chabrier-van Horn EOS [5].

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### P I.50

## Equation of state and phase diagram of ammonia at high pressures

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We present equation of state data as well as the phase diagram of ammonia at pressures up to 330 GPa and in the temperature range from 500 K to 10000 K. This regime is of great interest for interior models of the Giant Planets Uranus and Neptune which contain, besides water and methane, significant amounts of ammonia.

The equation of state data were obtained by ab initio simulations based on the Born-Oppenheimer approximation using the VASP code [1]. This method treats the electrons via finite-temperature density functional theory, whereas the ions are described within the framework of classical molecular dynamics.

The principal Hugoniot curve was derived from the equation of state and is in good agreement with experimental data. Furthermore, several other properties, such as pair distribution functions and diffusion coefficients, were calculated in order to construct the high-pressure phase diagram. In addition to a molecular and a dissociated phase, a rotationally disordered solid and a superionic phase were identified. Our predicted phase diagram shows several similarities compared to earlier work of Cavazzoni et al. [2]. Nevertheless, we obtain substantial deviations concerning the location and properties of the phases.

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#### P I.51

## Ab initio calculations for MgO at high pressures

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A large number of Super Earths, i.e. planets in the mass range 1-10  $M_{Earth}$ , have been discovered during the CoRoT and Kepler mission. The state of matter inside those planets (e.g. temperatures and pressures) is much more extreme that in the interior of the Earth.

In order to improve the understanding of the structure of exoplanets and their physical properties [1], ab initio calculations for their interior materials are needed. A possible representative is MgO, which is also an abundant material in the Earth mantle. Therefore, it is expected to be important for the mantle of exoplanets, as well as for giant gas planets with rocky cores such as Jupiter [2].

Using ab initio molecular dynamic simulations (VASP [3]), we have determined the phase diagram for MgO up to 14000 K and 1 TPa. In particular, the transition from solid state MgO to the liquid phase has been determined using diffusion analyses and

pair distribution functions. The transition from the NaCl- (B1) to the CsCl- (B2) structure of MgO is determined by calculating the respective free enthalpies. To determine the vibrational entropy, which is needed in the calculation process, phonon dispersions with Phonopy have been computed [4].

From the resulting simulation data the equation of state (EOS) is calculated and the Hugoniot curve is determined. The B1-to-B2-transition line, the liquid-solid transition line, and the phonon dispersion curves are compared with earlier simulation and experimental data.

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### P I.52

# Ab initio simulations for material properties along the isentrope of Jupiter

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The planet Jupiter contains matter under extreme pressures in the megabar regime and temperatures of several thousand Kelvin. Accurate knowledge about the behavior of the major constituents, hydrogen and helium, is required to model and understand the interior of Jupiter and other gas giant planets [1]. Transport properties like the thermal and electrical conductivity as well as the viscosity are particularly interesting to examine, since their behavior changes drastically at the transition from the dense nonideal plasma to the molecular fluid. Moreover, these quantities are a fundamental input in magneto-hydrodynamic simulations used to model the magnetic field of Jupiter [2]. The investigation of matter under extreme conditions is a challenge for both experiment and theory. We use ab initio molecular dynamics simulations to obtain equilibrium and transport properties. The method is based on a combination of finite-temperature density functional theory for the electrons with classical molecular dynamics for the ions [3]. This approach allows us to obtain equation of state data, phase diagrams, as well as transport and optical properties of warm dense matter with high accuracy.

Here we present new results [4] for thermodynamic material properties, the shear and longitudinal viscosity, the electrical and the thermal conductivity in hydrogen-helium mixtures along the isentrope of Jupiter, for which only relatively simple estimations are available so far. Our results cover the range from the outer molecular regions (2000 K, 5 kbar) to the core-mantle boundary (19000 K, 40 Mbar).

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These new data will lead, e.g., to significant improvements in understanding the origin and shape of the magnetic field of Jupiter.

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### P I.53

## Atmosphere and evolution of the young Hot Jupiter WASP-10b

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The atmosphere of a planet plays a major role in its evolution. Especially the atmospheres of close-in exoplanets receive a strong irradiation flux from their parent star, in addition to the infrared flux coming from the planet's interior. We implement the analytic atmosphere model from Guillot [2010] and calculate atmosphere models for the young Hot Jupiter WASP-10b. We connect our atmosphere models with a two-layer interior model consisting of a rocky core and an adiabatic envelope. With these models we perform evolution calculations. The comparison with the measured age of the star WASP-10 allows us to estimate the planet's present intrinsic temperature and its core mass. In addition to calculations with constant opacity ratio in the atmosphere, we construct model atmospheres that account for the pressure and temperature dependence of the opacities and investigate how these different atmospheres affect the evolution and derived core masses.

### P I.54

### Electric fields and currents in thunderclouds

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On any given day, there occur about 44000 thunderstorms on Earth. This is connected with the appearance of around eight million lightning strokes associated with currents of 200000 A. But up to now the physical mechanism of these phenomena is not yet finally clear. In the present contribution, the newly developed theory of cosmic ray shower-runaway breakdown in thunderclouds predicted by Gurevich et al. is reviewed. According to this theory, discharges in the cloud take place, when its maximum electric field is larger than the critical field for electron runaway. The critical field is about an order of magnitude smaller than the field of conventional atmospheric breakdown.

According to Gurevich, the runaway breakdown may be stimulated by cosmic ray secondary electrons. In this case the intensity of the breakdown is proportional to the energy of the cosmic ray particle. Due to collisions with air molecules, the fast runaway electrons generate new fast electrons, but also thermal ones. The number of the fast electrons in the atmospheric electron shower grows exponentially with both, the ratio of the maximum electric field to the critical one and the ratio of the altitudinal scale of the thundercloud electric field to the avalanche length. With the number of the electrons, also the electrical conductivity of the plasma and the electrical currents are changed. By the current changes, pulses of radio waves are generated which influence the signals received by VLF/LF radio stations as the station VADar of the University of Technology Darmstadt constructed to detect possible earthquake precursors in Europe. Here the modifications of the electrical conductivity by variations of the scales of the electric fields of the thunderclouds are estimated. First results are presented, which show the influence of lightnings on the European VLF/LF radio station network INFREP.

#### P I.55

## Application of the energy principle of ideal MHD to pinch plasmas

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Related to astrophysical and laboratory plasmas, it is very important to know if a plasma, in particular, a pinch one, is stable or not. And in case of laboratory plasmas, one has also to find out methods to avoid dangerous instabilities. Using the energy principle of magnetohydrodynamics (MHD), this all can be done without knowing the exact values of growth rates of instable waves. According to (A.N. Simakov, 2008), the growth rates of MHD instabilities in inertial fusion plasmas are, anyway, on the order or smaller than 5 percent of the possible observation times.

Applying the MHD energy principle means to analyse, if the potential energy of a plasma system may decrease for any of its allowable small displacements. If this is the case, the system is unstable. Thus, applying the MHD energy principle, one has to solve variational problems for the potential energy of the plasma.

The present work considers instabilities in plasmas with different plasma-wall boundary conditions, which may be described within the frame of ideal magnetohydrodynamics. For such problems, a considerable amount of analytical and numerical results (see e.g. (J.P. Freidberg 1982, K.-H. Spatschek 1990, Zdravkovich et al. 2001, P.A. Sturrock 2004)) already exists, which is here put into a common context.

Besides, some first steps are made to improve the recent theory taking into account non-axial-symmetry effects of the plasma in case of kink modes and considering the influence of gravity forces in astrophysics. Moreover, attempts are made to develop the energy principle for such anisotropic systems like planetary transition layers (e.g. the Earth's magnetosheath). For the case of internally homogeneous linear pinches, a system of equations for the vector of the displacement of the plasma is derived, which has to be solved numerically in future.

### P I.56

## Saturn's cooling history considering the demixing of hydrogen and helium

Robert Püstow<sup>1</sup>, Nadine Nettelmann<sup>1</sup>, Winfried Lorenzen<sup>1</sup>, Ronald Redmer<sup>1</sup>  $^1$  *University of Rostock* 

The source for the intrinsic excess luminosity in Saturn has been proposed to be helium rain for a long time. If we assume that Saturn evolved completely homogeneously its resulting cooling time is 2.2 billion years only. Compared to the age of the solar system of 4.56 billion years this is much to short because all planets are believed to have formed at the same time out of one protoplanetary disk. Therefore we present an inhomogeneous evolution model by considering the demixing of hydrogen and helium inside Saturn during its cooling history. This demixing effect leads to formation of helium droplets that fall into the planet's deeper interior and release gravitational energy. As a result we obtain a different energy budget and therefore a delayed cooling. Consequently we are able to prolong the cooling time of Saturn by considering this additional energy source inside the planet. We compare with earlier models that have been developed for this effect.



# Abstracts of posters: Session II Thursday 13.09.2012, 17:30 - 19:30

- ullet Statistical physics and ab-initio simulations Part 2
- Kinetics, transport and optical properties
- Ultra-intense laser-matter interaction
- Dusty plasmas

Nr.	Name	Title of contribution
P II.1	C. Caizergues	Frequency-dependent polarizability of atoms-in-jellium at finite temperature. Thomas-Fermi-Bloch model
P II.2	W. Ebeling	Electron transport mediated by solitonic excitations in plasma layers
P II.3	V.V. Karasiev	New finite-temperature orbital-free density functionals for warm and hot matter simulations
P II.4	S. Kyrkos	The roton minimum in dense plasmas
P II.5	A.V. Lankin	Influence of carbon materials structure on the formation of double layer in supercapacities
P II.6	L. Rajaei	The transmission wave from inhomogeneous over-dense plasma magnetized
P II.7	E. Apfelbaum	The electron transport coefficients of silicon and boron plasma
P II.8	Yu.V. Arkhipov	Optical properties of Kelbg-pseudopotential-modelled plasmas
P II.9	Y. Chen	Plasma diagnostics applying K-Line emission profiles of mid-Z materials
P II.10	R.I. Golyatina	Dependences of the diffusion and drift of helium ions in parent gas on its temperature
P II.11	D.V. Knyazev	Ab initio calculations of transport and optical properties of dense metal plasma
P II.12	S. Lorenzen	Quantum-statistical line shape calculations for dense H And H-like plasmas
P II.13	S.A. Maiorov	Effect of nonuniform electric field on diffusion and drift of electrons in gas
P II.14	B. Omar	Spectral line shapes in dense plasmas
P II.15	A.A. Ovechkin	Calculations of EOS and opacities of ionized matter using Liberman's model
P II.16	H. Reinholz	Dielectric function beyond RPA: kinetic theory vs. linear response theory
P II.17	I.M. Saitov	Atomistic modeling and simulation of warm dense matter in the two-temperature state
P II.18	N.A. Smirnov	Studies of absorbtion of femtosecond laser pulses in solid-density copper
P II.19	A.V. Sokolov	Optical characteristics of Coulomb systems
P II.20	K.M. Turekhanova	On the phenomenon of electron's runaway in partially ionized helium nonideal plasma
P II.21	M. Veysman	On the elaboration of a wide-range model for calculation of optical properties in warm dense matter
P II.22	K. Zemmour	FPLO ab initio estimate of electrical conductivity in nonideal copper plasma
P II.23	P.A. Zhilyaev	Ab-initio calculations of the thermal conductivity metals with hot electrons
P II.24	M. Arbeiter	Rare-gas clusters in intense VUV, XUV and soft x-ray pulses
P II.25	R.G. Bystryi	GPU-accelerated molecular dynamics simulations of ionized nanoclusters
P II.26	D. Komar	Control of photoelectron emission from metal clusters, exposed to intense few-cycle laser pulses
P II.27	S. Lochbrunner	Towards real-time characterization of plasma evolution induced by fs-laser pulses
P II.28	E.Yu. Loktionov	Femtosecond laser-induced gas-plasma flows optical, thermo physical and gas dynamic properties properties investigation for titanium targets irradiated in vacuum
P II.29	P. Mulser	Collisionless laser beam absorption
P II.30	C. Peltz	Attosecond plasma wave dynamics in laser-driven cluster nanoplasmas

Nr.	Name	Title of contribution
P II.31	S.P. Sadykova	Interaction of ultrarelativistic electron and proton bunches with
		dense plasmas
P II.32	V.A. Skvortsov	Computer simulation of energetic charged particles formation in
		laser plasmas
P II.33	N.I. Vogel	Ultra fast processes and evolution of structures of electric and
		magnetic fields in laser plasmas
P II.34	K. Walia	Effect of relativistic and ponderomotive nonlinearities on second harmonic generation
P II.35	A.E. Davletov	Influence of polarization phenomena on radial distribution function of dusty particles
P II.36	L.V. Deputatova	Electrodynamic confinement of dust particle at atmospheric conditions
P II.37	M. Djebli	Thermodynamical properties of finite two-dimensional dust clus-
1 11.07	Wi. Djebli	ters
P II.38	M.K. Dosbolayev	Structural and transport properties of dust formations in plasma
		gas mixtures in RF discharge
P II.39	L.G. D'yachkov	Clusters of diamagnetic dust particles in a cusp magnetic trap
		under microgravity conditions
P II.40	K.N. Dzhumagulova	On the diffusion and oscillations of the dust particles in the gas
D II 41	A 17 To:1:	discharge plasma
P II.41	A.V. Filippov	Shielding of the dust particle charge in a nonequilibrium plasma
P II.42	V.Yu. Karasev	Selection effect of dust particles by size and form factor
P II.43	S.I. Kopnin	Plasma-dust system in the surface layer of the illuminated part of
P II.44	V.I. Molotkov	the moon
P 11.44	V.1. IVIOIOTKOV	Motion of a projectile penetrating a dust crystal under microgravity
P II.45	V.I. Molotkov	Plasma crystals and liquids in experiments on the Internaional
		Space Station
P II.46	M.M. Muratov	The diagnostics of dusty plasma parameters on the basis of the
		microscopic properties
P II.47	S.A. Orazbayev	Spectroscopic diagnostics of plasma gas mixtures in radio fre-
		quency discharge
P II.48	A.A. Piskunov	Correlated motion of macroparticles in ordered dusty structure
P II.49	H. Thomsen	Phase transitions in spherical dust clusters: Analysis using the triple correlation function
P II.50	A.V. Timofeev	"Temperature" concept at description of dust particles dynamics
- 0		in gas discharge
P II.51	P. Tolias	The structure factor and critical point of weakly ionized dense
		dusty plasma systems
P II.52	Y.A. Ussenov	Study of the dust-free region near an electric probe in dusty plasma
P II.53	E.V. Vasilieva	Diagnostics of parameters of plasma in near-electrode area of RF-
		discharge under condition of dust monolayer
P II.54	L.M. Vasilyak	Glow discharge positive column with dust particles in neon

### Statistical physics and ab-initio simulations – Part 2

### P II.1

# Frequency-dependent polarizability of atoms-in-jellium at finite temperature. Thomas-Fermi-Bloch model

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The frequency-dependent polarizability (FDP) of a plasma is a key quantity directly related to photo-absorption cross section and conductivity. We report on calculation of the FDP from the linear response theory in case of plasmas composed of continuum electrons and ions that have bound electrons. Plasma equilibrium is treated in the framework of our variational-average-atom-in-quantum-plasma (VAAQP) approach [1,2]. At present we calculate FDP in the simplest Thomas-Fermi (TF) version of the VAAQP model using Bloch hydrodynamics (TF-Bloch) approach, similarly as in Ref. [3] which allows us to account self-consistently for the induced frequencydependent density and electric potential. A new sum rule, originally proposed in the fully quantum VAAQP [4], was proved in the TF-Bloch formalism and for the first time checked in our numerical calculations. The FDP and the sum rule provide information on the importance of the induced density and electric field on plasma photo-absorption and conductivity. The TF-Bloch case allows us to have a direct insight into the rather involved mathematics of the self-consistent FDP calculations in the situation when non-homogeneous central atom and its plasma vicinity are both perturbed by an electric field.

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#### PII.2

# Electron transport mediated by solitonic excitations in plasma layers

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We study plasma transport coupled to soliton-like excitations in layers of atoms interacting by Morse forces. Including interactions with the imbedded electrons we investigate the bound states between charges and solitonic excitations, called solectrons. The atomic dynamics is given by nonlinear classical Langevin equations including nonlinear couplings and sources of noise. It is shown that solitonic excitations are of particular high stability against perturbations move with sound velocity. The dynamics of free imbedded charges (electrons) is modelled in the framework of tight-binding approximations and stochastic master equations. Assuming that the charges are attracted by local compressions it is shown that rather stable bound states between charges and soliton-like excitations are formed, which can carry electricity with sound velocity. We study the dynamics of these quasiparticles, which move in general with supersonic velocity and are called solectrons, in dependence on noise/temperature and study possibilities of control. Further we study pair formation. Several applications including the interpretation of the observed high drift velocity in polydiacetylen, the observed excitations in cuprate layers and the control of electron transfer by acoustic excitation of at the nano-scale are discussed.

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### P II.3

## New finite-temperature orbital-free density functionals for warm and hot matter simulations

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Finite-temperature density functional theory (ftDFT) for the electrons combined with classical mechanics for the ions is a standard approach to treat warm dense matter. Usually ftDFT is implemented via the orbital-dependent Kohn-Sham (KS) procedure. KS computational cost scales as the third or higher power of the electron number at zero temperature and worsens with increasing temperature because of the growing number of partially occupied orbitals which must be included. Orbital free finite-temperature DFT (of-ftDFT) in principle provides the same quantum-mechanical treatment at a computational cost which scales as the system volume and is temperature independent.

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The main ingredient of-ftDFT is the non-interacting free energy density functional. Its two largest components are the non-interacting kinetic energy and entropy. The only two non-interacting free-energy functionals proposed in the literature and used thus far in of-ftDFT calculations are the finite-temperature Thomas-Fermi (ftTF) functional (Feynman et al., 1949) and ftTF with gradient-corrections, equivalent to the finite-temperature second-order gradient approximation (ftSGA) (Perrot, 1979). In the present work we report new finite-temperature generalized gradient approximations (ftGGA) for the non-interacting free energy functional. The finite-temperature extensions of known zero-temperature kinetic energy functionals in framework of ftGGA are constructed. Results (total free energies and pressure) from these new ftGGA functionals show much better agreement with the reference Kohn-Sham values as compared to the ftTF and ftSGA values. Other issues related to of-DFT methods such as development of local model potentials and production of reference data to calibrate temperature-dependent density functionals (including the exchange free energy) also will be discussed.

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### P II.4

### The roton minimum in dense plasmas

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Electric double layer is studied on the border between an activated carbon electrode and electrolyte aqueous solution. Quantum molecular dynamics in the DFT approximation is used. The results show that it is electron-hole electric double layer in the near electrode bulk activated carbon that is a prevailing factor in the formation of the total system capacity. It is connected with the relatively low number density of charge carriers in the carbon materials with respect to the ion number density in electrolyte. The influence of the peculiarities of the geometric and electron structure of the activated carbon is analyzed. In particular the importance of admixtures in carbon is considered. Layered clathrate formation is treated. The main consideration is given to the implantation of metals of the IA and IB subgroups. It is shown that the implantation results mostly in the increase of the system capacity.

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#### PII.5

### Influence of carbon materials structure on the formation of double layer in supercapacities

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Electric double layer is studied on the border between an activated carbon electrode and electrolyte aqueous solution. Quantum molecular dynamics in the DFT approximation is used. The results show that it is electron-hole electric double layer in the near electrode bulk activated carbon that is a prevailing factor in the formation of the total system capacity. It is connected with the relatively low number density of charge carriers in the carbon materials with respect to the ion number density in electrolyte. The influence of the peculiarities of the geometric and electron structure of the activated carbon is analyzed. In particular the importance of admixtures in carbon is considered. Layered clathrate formation is treated. The main consideration is given to the implantation of metals of the IA and IB subgroups. It is shown that the implantation results mostly in the increase of the system capacity.

### P II.6

# The transmission wave from inhomogeneous over-dense plasma magnetized

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The high transparency condition of an overcritical plasma layer due to the excitation of electromagnetic surface modes was studied. One of the simplest model to describe of this procedure is that the plasma is sandwiched between two dielectric layer. Our studies are classified in two groups . The first, the penetration of an electromagnetic wave in an inhomogeneous over-dense plasma is studied. It is shown that surface Plasmon is excited without present of dielectric layer also the effect of inhomogeneity on transmission wave from this layer is investigated. The second, it is considered that the inhomogeneous over-dense plasma is immersed in a magnetic field. Then how to affect magnetic field on transmission wave is analyzed.

## Kinetics, transport and optical properties

### P II.7

## The electron transport coefficients of silicon and boron plasma

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The electron transport coefficients of various substances have been investigated more than a century in theory and experiments. The region of dense plasmas possibly is the most problematic one in these studies. At T>5-10 kK and densities less than normal one there are little measurements. Besides the theoretical approaches developed in very dense (solid) and very rarefied (gas) phases are inapplicable directly in this area. But during last two decades new measurements in high-temperature region for various substances have appeared. In particular the electrical conductivity of silicon and boron has been measured recently in the wire explosion experiments. In present work we apply the generalized chemical model to calculate the conductivity, thermal conductivity and thermal power for these two elements in plasma state. Earlier this model was successfully applied to calculate the composition and conductivity of the noble gases and noble metals plasmas. The results of calculation have been compared with available data of measurements and calculations.

### P II.8

## Optical properties of Kelbg-pseudopotential-modelled plasmas

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The simulation data [1,2] on hydrogen-like plasmas modelled with the Kelbg pseudopotential are treated within the classical theory of moments. It is shown that the model data on the inverse dielectric function satisfy five convergent sum rules and other exact relations. The sum rules which are the power frequency moments of the loss function are calculated using the Kelbg potential and the Ornstein-Zernike hypernetted-chain equations. An approach to the reconstruction of the Nevanlinna parameter function is suggested and successfully tested. The long-wavelength model plasma oscillations are studied. Conclusions with respect to the applicability of the Kelbg potential are drawn.

Acknowledgment. This work was partially supported by the Ministry of Education and Science of the Republic of Kazakhstan under Grants No. IPC 11/2012, ITT 02/2012 and the Spanish Ministerio de Ciencia e Innovacion under Grant No. ENE2010-21116-C02-02. The authors acknowledge the financial support of KazNU; I. M. T. is grateful

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### PII.9

## Plasma diagnostics applying K-Line emission profiles of mid-Z materials

Yiling Chen<sup>1</sup>, Heidi Reinholz<sup>1</sup>, Gerd Röpke<sup>1</sup>

Theoretical treatment of spectral line shifts is applied to various moderately ionized mid-Z materials. We focus on the opposing influence of ionization/excitation (blue shift) and plasma polarization effects (red shift). Recent results on silicon (semi-conductor) consider the different configurations of the emitting Si ion  $(1s^12s^22p^{\alpha}, \alpha = 6, 5, 4)$  that corresponds to  $K\alpha L^N$ , N = 0, 1, 2. In order to observe  $K\alpha L^N$  lines, we use gaussian 03 codes to calculate the atomic states. Synthetic spectra have been evaluated and compared with experimental data [1]. As the  $K\alpha LN$  spectra are emitted from a silicon plasma we are able to infer plasma parameters by studying the line profiles [2].

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### P II.10

# Dependences of the diffusion and drift of helium ions in parent gas on its temperature

S.N. Antipov<sup>1</sup>, R.I. Golyatina<sup>2</sup>, S.A. Maiorov<sup>2</sup>

In this presentation we consider the drift of helium ions in a gas in a uniform electric field. Model ion collisions, which implemented in the Monte Carlo method, allows you properly account the energy balance of ions during their drift. The calculations are performed for gas temperatures in the range 1 to 1000 K and various reduced electric field:  $E/N=10,\,30,\,100$  Td. The tables shows the temperature series of the gas atoms, the ion drift velocity, the effective temperature of the ions, defined as two-thirds

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of the average energy, transverse and longitudinal temperatures, the diffusion coefficients along and transverse to the direction of the field, the mean free path of ions, and part of collisions with back scattering to the total number of collisions. Note that usually there given the experimental and calculated data for the drift velocity, but for a correct analysis of the gas discharge there are needed other kinetic characteristics of ion drift. These calculations can be used in the analysis and design of experiments with dusty plasmas in a cryogenic discharge.

### P II.11

# Ab initio calculations of transport and optical properties of dense metal plasma

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Ab initio calculation of dynamic electrical conductivity, thermal conductivity and optical properties of dense metal plasma (aluminium, silver) was performed in this work. The calculation is based on quantum molecular dynamics (QMD) and density functional theory (DFT).

QMD simulation is used to calculate time evolution of ionic subsystem. Independent ionic configurations are selected from the equilibrium section of the molecular dynamics run for the calculation of transport properties. Detailed zone structure calculation is performed for each of these configurations. Electronic energy levels and wave functions are obtained and then used to calculate the Onsager coefficients using the Kubo-Greenwood formula in the Chester-Thellung version [1]. The values of the Onsager coefficients for different ionic configurations are averaged. The static values of electrical and thermal conductivities are calculated by the extrapolation of the Onsager coefficients to the zero frequency. The imaginary part of electrical conductivity is obtained via the Kramers-Kronig transformation. Then optical properties are calculated: complex dielectric function, complex refractive index, reflectivity and opacity. QMD simulation and electronic structure calculation are performed using Vienna Ab initio Simulation Package (VASP) [2].

The calculation is performed for aluminium and silver at different temperatures and densities in solid and liquid phase. Particular attention is devoted to the near-normal densities for temperatures from normal up to 20000 K. The convergence of the results with the parameters of the calculation is examined. The results are compared with data of other authors, reference and experimental data.

The calculations of this work were used to calibrate the semiempirical models of dielectric function and thermal conductivity necessary for the simulation of femtosecond laser interaction with matter.

This work is supported by FAIR-Russia Research Center grant for master students (2011-2012) and JIHT RAS Young Scientists Support Fund.

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### P II.12

# Quantum-statistical line shape calculations for dense H And H-like plasmas

Sonja Lorenzen<sup>1</sup>, Heidi Reinholz<sup>1</sup>, Gerd Röpke<sup>1</sup>, Mark C. Zammit<sup>2</sup>, Dmitry V. Fursa<sup>2</sup>, Igor Bray<sup>2</sup>

In this contribution, we present results for the Lyman lines of hydrogen and hydrogenlike ions in dense plasmas. Full line profiles are calculated within a quantum-statistical method, based on thermodynamic Green's functions. The focus is on the contribution to broadening and shift due to free electrons beyond the Born approximation.

The self-energies of initial and final state are central quantities in the Green's function method. The real and imaginary part of the self-energy correspond to the shift and broadening of the energy levels due to the surrounding medium, respectively. Ions and electrons are treated separately. As we consider the influence of surrounding ions in quasi-static approximation, the ionic self-energy is given by the linear and quadratic Stark effect. The electronic self-energy is calculated within a quantum-statistical manybody approach based on thermodynamic Green's functions. The Born approximation has often been applied to give a perturbative approximation for the electronic selfenergy [1,2]. However, in dense plasmas, strong electron radiator collisions are relevant and have to be included, too. The effect of strong collisions can be identified as ladder-like diagrams of the electron-emitter propagator. In an effective two-particle approximation the electronic self-energy is given in terms of scattering amplitudes [3], analogously to Baranger's expressions for line shift and broadening [4]. Here, we use scattering amplitudes obtained from close-coupling calculations [5]. The isolated scattering of an electron with the emitter does not allow for medium effects. To include the screening due to free electrons in the plasma, Debye screening is implemented into the close-coupling calculations [6].

In our examples, the free electron density ranges between  $10^{23}$  and  $10^{26}$  m<sup>-3</sup> and the temperature is between  $10^4$  and  $10^6$  K.

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### P II.13

# Effect of nonuniform electric field on diffusion and drift of electrons in gas

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In considering the various tasks associated with the drift of electrons in gas discharge plasma is often assumed that the drift velocity and drift characteristics in each point of space (the average energy, diffusion coefficients, the ionization energy and the Townsend coefficient) depend only on the electric field and gas density (or from the reduced field E/N) at this point. However, many phenomena in physics, a gas discharge plasma due to the effect of non-locality, when the characteristics of electron gas at a given point depends on the parameters of the electron gas in other poins.

In this paper we consider the drift of electrons in a given non-uniform periodic electric field of the two species. The first type of field - a sinusoidal field, a second type of field - a sawtooth.

To investigate the effects of non-locality the solution of the motion equations for the swarm of electrons, not interacting with each other was carried out. Collision of electrons with atoms taken into account by the Monte Carlo method (MC). This MC method taken into account the dependence of cross sections of elastic collisions on the velocity, energy loss of electrons by atomic excitation, ionization, appearance of new electrons with a nonzero energy, loss of electrons at the walls due to potential barrier wall.

On the basis of runs was investigated the influence of field inhomogeneity on the general characteristics of drift (mean electron energy, drift velocity, Townsend ionization coefficient, etc.). Also was investigated the effect on the function of the electron energy distribution following parameters of the problem - the period and the magnitude of the fluctuations of the field at a fixed average field. Were also calculated the characteristics of spatial distribution on the field period (striations). It was found that increasing the degree of inhomogeneity of field leads to a decrease in the average electron energy, reduce its drift velocity and an increase of ionization rate.

### P II.14

## Spectral line shapes in dense plasmas

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Spectral line broadening is investigated for singly charged ions, based on a microscopic quantum statistical approach in dense plasmas. By using thermodynamic Green's function, perturber-radiator interaction, plasma correlation and screening effects are taken into account. Ions are treated in quasistatic approximation, leading to Stark

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effect in the surrounding perturbers microfield. A T-matrix approach is used to improve semiempirical cut-off procedure for describing radiator-electron strong collisions. Stark broadening for  $(2p^3P_{2,1,0}\text{-}2s^3S_1)$  transition of helium-like lithium is calculated, plasma parameters such as spatial- temperature and electron density for the expanding Li plasma after 60 ns from laser irradiation are analyzed. The estimaed spatial electron density and temperature ranges are  $n_e{=}(0.25\text{-}2)\times10^{24}~\text{m}^{-3}$  and  $T\approx(2\text{-}3.5)~\text{eV},$  respectively. The dependence of plasma parameters on the line width are investigated. A good agreement is shown by comparing the calculated values with the available measured profiles.

#### P II.15

### Calculations of EOS and opacities of ionized matter using Liberman's model

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An important feature of the average atom models [1] stems from the fact that those allow one to simulate thermodynamic, optical, and transport properties of pure elements and mixtures in wide temperature and density domains on the base of the same theoretical footing. Recently, the RESEOS code [3] originally developed for the EOS calculations by using Liberman's model [4] was extended by implementing the superconfiguration approach [2] to simulate spectral-line photoabsorption. The presentation provides comparisons of calculated EOSs, shock Hugoniots, and opacities with other experimental and theoretical data. Special attention is paid to the sensitivity of thermodynamic functions to the temperature dependence of local exchange potential and to the smoothness of the opacity dependence on the material density under the pressure ionization. A generalization of the superconfiguration concept [2] is also formulated. This generalization is shown to be equivalent to the employment of an effective method of accounting for the occupancy fluctuations for a number of atomic subshells [5] thus enabling one to reduce the amount of spectral lines taken into account at an appropriate accuracy of the modeled absorption and emission spectra.

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#### P II.16

# Dielectric function beyond RPA: kinetic theory vs. linear response theory

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Calculating the frequency dependent dielectric function for strongly coupled plasmas, the relations within kinetic theory and linear response theory are derived and discussed in comparison. In this context, we give a proof that the Kohler variational principle can be extended to arbitrary frequencies. It is shown to be a special case of the Zubarev method for the construction of a non-equilibrium statistical operator from the principle of the extremum of entropy production. Within kinetic theory, the commonly used energy dependent relaxation time approach is strictly valid only for the Lorentz plasma in the static case. It is compared with the result from linear response theory that includes electron-electron interactions and applies for arbitrary frequencies, including bremsstrahlung emission. It is shown how a general approach to linear response encompasses the different approximations and opens options for systematic improvements.

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### P II.17

# Atomistic modeling and simulation of warm dense matter in the two-temperature state

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Warm dense matter (WDM) is an intermediate state between the heated condensed matter and plasma. In other words the WDM state possesses both crystal and plasma properties. The correct theoretical description of such a state is not yet developed. The attempts to extrapolate the existing theories of plasma and condensed matter to this region are questionable. The importance of the development of WDM theoretical description is determined by the fact that such conditions may arise in the variety of different scientific and industrial applications. For instance, WDM is formed: in the matter impacted by femto- and picoseconds laser pulses; in nuclear materials at the formation of radiation track, exploding wires, cathode erosion at high current pulses etc. The system is in the two-temperature state initially, the electronic temperature being several orders higher than the ionic one in these phenomena.

A model of WDM and its relaxation is developed in this work. The ion and electron subsystems are described in different approximations. The electron-phonon relaxation is taken into account for both subsystems with the same coupling.

The first set of equations describes the ion subsystem by means of classical molecular dynamics of ions. We propose the two-temperature atomistic approach with an

electron-temperature-dependent (ETD) interionic potential. Since the electron temperature depends on time, the interionic potential depends on time in an implicit way. The use of ETD-potential makes it possible to take into account the influence of the electronic pressure on the behavior of ions. Langevin thermostat is used for the electron-ion relaxation. All the properties are taken for the bulk matter. It is shown that the free surface and the double layer formation at ablation do not influence the results significantly. DFT is used for this problem.

Another equation treats the relaxation of the electronic subsystem which is considered in the continuum approach. Electron thermal conductivity is calculated in the DFT approximation. Source of initial heating is included into the equation for the laser ablation. Initial conditions are taken in the form of the initial distribution of the electron temperature for the task of track formation.

The various processes are simulated with the use of the model developed: melting and ablation of metals at laser pulse irradiation, formation of tracks by swift heavy ions in nuclear materials. Comparisons to the experimental data are performed.

### P II.18

# Studies of absorbtion of femtosecond laser pulses in solid-density copper

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We performed theoretical and experimental studies of absorption of 800 nm normal-incidence femtosecond laser pulses by a metal copper target. Numerical simulation was performed with a modified version of the 1D ERA hydrocode [1] that employs new theoretical data on thermodynamic functions of the target material along with an improved description of relaxation and electron-ion energy exchange rates. These new data were obtained within the density functional theory using the modified full-potential linear muffin-tin orbital method (FP-LMTO) [2,3], Liberman's model [4] implemented in the RESEOS code [5], and a chemical-picture-based model of dense plasmas utilizing the superconfiguration approximation (CPSC) [6].

The measurements of laser-pulse absorption coefficients A(IL) in copper were performed on the RFNC-VNIITF femtosecond laser facility in the range of laser light intensities on the target IL  $\sim 10^{12}$ – $10^{15}$  W/cm<sup>2</sup>. We present the layout of the experiments and the comparisons of theoretical dependences A(IL) with the results of measurements and with the other theoretical and experimental data [7,8]. We also analyze the role of the electron-ion energy exchange and the effect of metal-bond hardening in copper heated by femtosecond laser pulses.

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### P II.19

## **Optical characteristics of Coulomb systems**

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One problem of plasma physics, which cannot be considered as completely solved is the determination of high-frequency (optical) complex conductivity of dense plasmas at moderate  $\sim \! 10000$  K temperatures. The classical Drude formula for the complex conductivity though well operating over wide ranges of temperatures and particle densities needs in general quantum corrections. The simplest of those is subject to the non-zero probability that electron and ion are localized at the same point. We investigate a modified Drude expression found in the one-electron approximation with account of the above correction using as tools the method of Green functions, the theory of moments and the method of pseudo-potentials.

In addition we specify the simple expression for static conductivity of Coulomb systems through transport section of electrons on ions by appropriate choice of ions pseudo-potentials. In doing so we take into account possible bound states of conductivity electrons on ions.

### P II.20

# On the phenomenon of electron's runaway in partially ionized helium nonideal plasma

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The investigation of epithermal and runaway electrons in tokomaks and stellarators is actually in program of controlled thermonuclear fusion. The runaway electrons effect significantly to profile current in installations with magnetic confinement, and it adversely affect to the stability of the plasma [1,2]. Therefore, there is a need to develop the experimental and theoretical methods control the number and energy of runaway electrons produced during disruptions [3,4]. In this work we continue to develop the theory of runaway electron's phenomenon.

This work is devoted to the investigation of effect of runaway electrons in partially ionized helium dense plasma using the effective potentials of particle's interaction [5,6]. At the investigation of composition of plasma we used the Saha equation with corrections to nonideality (lowering of ionization potentials).

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The conditions of runaway electrons were determined, and it compared with other approximations.

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### P II.21

# On the elaboration of a wide-range model for calculation of optical properties in warm dense matter

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Optical properties of warm dens matter irradiated by laser radiation are studded by means of both kinetic and quantum statistical (QS) approaches for wide range of plasma (temperatures and densities) and laser (frequencies) parameters.

It is demonstrated, that both approaches give the same results for weakly-coupled plasmas and for optical laser frequencies. In the region of low (in comparison with effective frequencies of electrons collisions) frequencies of laser radiation it is demonstrated, that QS theory, based on the calculations of J-J correlation functions within one-moment approach, underestimates the values of plasma permittivity, and higher-order moments of electron distribution function should be used in calculations of correlation functions. Classical kinetic theory can be applied for laser frequencies below than plasma frequency. At higher frequencies the QS theory within screened Born or Lennard-Balescu approximations can be applied. It is demonstrated, that at high frequencies QS theory gives results similar to that obtained from the theory of bremsstrahlung radiation and detailed balance principle. The advantage of QS theory is it's wider range of applicability and possibility to consistently take into account screening, correlations, and strong coupling effects.

In the region of strongly coupled non-degenerate plasmas (for solid-density aluminum the corresponding electronic temperatures are from about 20 till 200 eV), the kinetic approach with Rutherford electron-ion collision cross-section underestimates the values of effective collisional frequency and imaginary part of plasma permittivity, in comparison with the QS approach. This is connected to the fact that Rutherford-like cross-sections don't take into account strong collisions with electron scattering on the large angles, which are essential in the region of strong coupling. Such collisions can be taken into account in QS theory by means of T-matrix approach.

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The interpolation formulas for wide-range permittivity of warm dens matter are suggested.

### P II.22

# FPLO ab initio estimate of electrical conductivity in nonideal copper plasma

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We present an ab initio calculation of the electrical conductivity of nonideal copper plasma. The electronic energy is computed using, in the framework of the density functional theory (DFT), the method of the Full-Potential non-orthogonal Local-Orbital Minimum-Basis Band-structure Scheme (FPLO) in the local spin density approximation with the on-site Coulomb interaction (LSDA+U) and the coherent potential approximation (CPA). The comparison of our ab initio calculations with different theoretical and experimental results is carried out. The calculated electrical conductivity agrees qualitatively with that obtained theoretically by Zaghloul and experimentally. Our results suggest that the FPLO ab initio approach is sufficient to allow approximate calculations of the electrical conductivity.

### P II.23

# Ab-initio calculations of the thermal conductivity metals with hot electrons

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The interaction of ultra-short laser with metal result in the two-temperature (2T) state in which the temperature of the electronic subsystem (Te) by orders of magnitude greater than the ion temperature. Description of 2T state is important for understanding the mechanisms of laser ablation, since at this stage number of relevant phenomenon occurs: transfer of laser energy to the ions, creation of warm layer which determine the future dynamics of the system. The numerical simulation of laser ablation requires the kinetic coefficients of the metal with hot electrons. However, phenomenological dependencies are mostly used with contains adjustable parameters determined from the asymptotic behavior at low and high Te. Ab-initio methods don't have such deficiencies, because there are no adjustable cofficient. This paper presents an ab-initio calculation of the thermal conductivity of the metal with hot electrons, calculated from the Kubo-Greenwood formula. The calculation is performed for liquid aluminum in the range of Te from 0 to 6 eV. The dependence of thermal conductivity is in a good agreement with calculations from kinetic equation.

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### Ultra-intense laser-matter interaction

### P II.24

## Rare-gas clusters in intense VUV, XUV and soft x-ray pulses

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We investigate the wavelength dependent ionization, heating, and expansion dynamics of medium-sized rare-gas clusters (Ar<sub>N</sub>) under in- tense femtosecond short-wavelength free electron laser pulses by quasi-classical molecular dynamics simulations. A comparison of the interaction dynamics for pulses with  $\hbar\omega$ =20, 38, and 90 eV photon energy at fixed total excitation energy indicates a smooth transition from plasma-driven cluster expansion, where predominantly surface ions are expelled by hydrodynamic forces, to quasi-electrostatic behavior with almost pure Coulomb explosion[1]. Corresponding signatures in the time-dependent cluster dynamics as well as in the final ion and electron spectra support that this transition is linked to a crossover in the electron emission processes. This would be of interest for applications that are closely related to the correlation between ionization and expansion dynamics of many-particle systems in intense FEL pulses, such as single-shot diffractive imaging or time resolved x-ray holography.

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### P II.25

## GPU-accelerated molecular dynamics simulations of ionized nanoclusters

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Irradiation of nanosized metallic clusters by femtosecond laser pulses of moderate intensities  $(10^{13} - 10^{16} \text{ W/cm}^2)$  has been considered recently in both experiments and computer simulations [1]. It has been shown that the plasma generated by ionization of cluster atoms is nonideal which allows one to apply these studies to the development of nonideal plasma theory. Electron plasma oscillations, electron-ion collisions, relaxation rates in such nanoplasma are of particular interest in view the size effects essential for the cluster plasma [2,3].

The method of molecular dynamics (MD) is probably the most suitable numerical technique to study dynamical processes in the cluster nanoplasma due to a small number of particles. However, the long-range type of Coulomb interaction requires calculation of the full interaction matrix and disables the conventional optimization techniques routinely used for the short-range potentials. Alternatively one can use Tree-MD or

PPPM approximations but nevertheless the simulations time scales too rapidly with the number of particles. It constitutes a problem of simulating the systems of intermediate size between cluster and bulk plasmas.

In this work we propose to use the Graphics Processing Units (GPUs) to accelerate MD simulations of the nonideal nanoplasma. Contemporary GPUs are widely used for scientific computing and showed their high efficiency for a particular class of atomistic simulations [4]. In our case it results in the speedup of two orders of magnitude when comparing Nvidia Tesla M2050 GPU and a single core of Intel Xeon E5520 CPU. It allows us to increase the number of particles and observe the transition of the electron oscillation spectra in the cluster plasma ranging from 55 to 10<sup>5</sup> ions. The dependence of frequency and damping of different collective plasma oscillation modes including Mie and Langmuir oscillations are presented.

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### P II.26

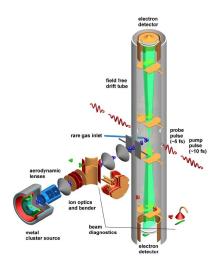
## Control of photoelectron emission from metal clusters, exposed to intense few-cycle laser pulses

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Collective electron motion induces strong polarization fields in metal clusters exposed to intense optical pulses. Highly charged and energetic species are generated by resonant excitation of the cluster plasmon mode via an optimized pump-probe sequence. We conducted first pump-probe experiments on metal clusters exposed to  $\omega-2\omega$  and few-cycle laser pulses. A time of flight electron spectrometer allows to register emission in both directions of the laser polarization axis (see figure below). Electron spectra from few-nm sized silver particles exceeding 1keV (100 Up) at laser intensities of only  $10^{14}$  W/cm<sup>2</sup> were obtained. By using the single-shot carrier-envelope phase (CEP) technique, the dependence of the directional emission with respect to CEP has been studied. Strong anisotropies of re-scattered electrons have been obtained. Moreover, asymmetric pulses allow to control energetic electron emission on a sub-cycletime scale.

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P II.27

# Towards real-time characterization of plasma evolution induced by fs-laser pulses

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Femtosecond-laser ablation is considered as a unique technique for material processing that gives the opportunity for precise micromachining, material synthesis, growth of thin film and others. Such a wide range of technological applications stimulates the interest in the physical processes that accompany laser ablation. When an intense ultrashort laser pulse hits opaque condensed matter, the laser radiation is absorbed within a thin layer of the material and the electromagnetic energy is converted into electronic excitations. If the energy absorbed by the electrons exceeds the Fermi energy, the electrons can escape from the target. The electric field due to the resulting charge separation pulls also the ions out of the target. Obviously, the major processes during laser-matter interaction that influence the ablation results are electron heating by the laser field and the following complex electron dynamics. In case of fslaser-matter interaction the material properties such as electron number density and therefore the plasma frequency, the absorption coefficient, and others depend strongly on the parameters of the applied laser field. One of the possibilities to achieve flexible control of the laser matter interaction is shaping of the laser pulse in amplitude and phase.

To observe the time dependent material response on the impact of a laser pulse, we have developed a pump-probe setup utilizing transmission and diffraction of an ultraviolet probe beam. NIR pulses at 800 nm with a duration of 50 fs are supplied by a regenerative Ti:Sapphire amplifier system. One part of the NIR beam passes a 4f-pulse shaper based on a liquid crystal mask to provide excitation pulses whose temporal shape can be varied. A second fraction of the NIR beam is guided via a computer controlled delay stage and then frequency doubled to generate probe pulses in the near UV. The excitation and the probe beam are collinearly focused onto a target foil. The probe light transmitted through the foil is recorded by a CCD camera in dependence on the delay time between excitation and probe pulses. Here we present first results on the time dependent sample transmission and discuss the findings with respect to

the plasma evolution. The influence of the temporal structure of the excitation field will be investigated by shaping the pump pulse.

### P II.28

### Femtosecond laser-induced gas-plasma flows optical, thermo physical and gas dynamic properties investigation for titanium targets irradiated in vacuum

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Titanium femtosecond laser ablation spectral thresholds are lower than those for the most of refractory metals, considering its wide technological application, ultrashort laser pulses interaction with Ti-targets investigation is of great interest. Commonly used diagnostical tools such as atomic emission spectroscopy or shadowgraphy provide poor, often semi-quantitative or just qualitative data. Using specially developed target surface and near-surface region combined interferometry and complex data processing techniques (with spatial ~10-6 m and temporal ~10-13 s resolution for  $\delta t$ >10-11 s) laser-induced ( $\tau$  ~45, 60 fs,  $\lambda$  400, 800 nm, I0,max~ 2.5 · 10<sup>14</sup>, 9.4 · 10<sup>15</sup> W/cm<sup>2</sup>, pamb~ 5 · 10<sup>-4</sup> mbar) Ti plasma plume optical, thermo physical and gas dynamic properties dspatio-temporal distribution have been obtained.

The method is based on combining data regarding to plume refraction and absorption k indices and target mass flow rate  $\delta m$  ( $\delta m/Elas 0.02-0.08 mg/J$ ). Assuming electron contribution as dominating for refraction index formation and plume as axis symmetrical electron concentration ( $n_e \sim 10^{18} - 10^{20} \text{ cm}^{-3}$ ) was calculated, using ne as weight function for particles local concentration velocity distribution and mean velocity ( $\langle v \rangle \sim 3.5 - 8.5 \text{ km/s}$ ). Relation between electron concentration volume integral and number of particles derived from mass flow rate gives evaluation of plume ionization rate, which reaches  $\varepsilon \sim 2$ . Temperature can be estimated using Kramers-Unsold formula, assuming LTE conditions, and using data on local absorption coefficient ( $k\sim4-400$  cm<sup>-1</sup>), ion and electron concentration, obtained values are T $\sim0.7-5$ eV. These data are in good agreement with published results for close experimental conditions. Unique results refer to static p $\sim$ 105-108 Pa and total pressure p\* $\sim$ 106-1011 Pa distributions, close results were previously obtained theoretically only. Other results regard to gas-plasma flow generation efficiency such as momentum coupling coefficient reaching Cm $\sim 1.8 \cdot 10^{-4}$  N/W, energy  $\eta = \delta \text{m} < \text{v} > ^2/2 \text{Ela} \sim 0.12 \cdot 0.37$  and thrust  $\mu = \langle v \rangle^2 / \langle v^2 \rangle \sim 0.6$ -0.93 efficiency. Presented results, which are in good agreement with experimental and theoretical reference data, provide a detailed and highly resolved quantitative characterization of laser-induced Ti plasma plume needed for a wide range of applications processes optimization.

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### P II.29

### Collisionless laser beam absorption

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After nearly three decades of research on superintense laser-dense matter interaction collisionless absorption is still not sufficiently understood. Estimates show that from intensities of  $I=10^{16}\,\mathrm{W/cm^2}$  on collisional absorption becomes inefficient; the excellent conversion efficiency at relativistic and subrelativistic irradiances under p-polarization, demonstrated by experiments and simulations, has to rely on collisionless processes. Various mechanisms and models have been proposed, from anomalous skin effect, vacuum heating and wave breaking to Landau damping. The models are either based on simulations only (e.g., j x B heating) or they are in disagreement with basic experimental or simulation results.

The experiments and simulations show the splitting of the heated electrons into a low energy group and a high energetic Maxwellian tail, however they do not tell which are the leading physical mechanisms responsible for it. They need interpretation. A detailed analysis shows that the so-called Brunel mechanism [1] explains essential aspects of collisionless absorption: prompt generation of electrons during one laser cycle or a fraction of it, decay into two groups, insensitivity of absorption with respect to target density well above critical. Such positive aspects contrast with a non-Maxwellian tail of the hot electrons, too low energy cutoff, excessively high fraction of fast electrons, scaling of mean electron energy with laser intensity drastically differing from experimental and other analytical findings in the current literature [2]. A fundamental question arises: What is the essential part of physics missing in Brunel's and analogous models?

Partial answer to the question may come from an alternative model that is based on anharmonic resonance [3] and modifications of it at superintense laser fields [4]. In contrast to [1] in this model the individual electron layers are allowed to undergo several oscillations before being driven into local resonance by the laser field and then escaping into the cold target in a disruption-like manner. Owing to the dynamic phase shift associated with resonance a very efficient breaking of flow ("resonant breaking") and mixing of layers takes place. Mixing produces stochastic motion, longer life time in front of the target, Maxwellization and fast tail formation in the energetic electron spectrum as well as a natural reduction of the electron reentry currents and, in concomitance, the decrease of fraction of their number down to a few percent. It will be shown to what extent the two models [1] and [3] compete with each other and which changes in the scaling laws compared to [2] will follow from their interplay in the various laser intensity regimes.

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### P II.30

# Attosecond plasma wave dynamics in laser-driven cluster nanoplasmas

Christian Peltz<sup>1</sup>, Thomas Fennel<sup>1</sup>, Charles Varin<sup>2</sup>, Thomas Brabec<sup>2</sup>

Molecular dynamics (MD) and particle-in-cell (PIC) methods have been used with great success for modeling intense laser-plasma interaction, though both have certain important limitations. Electrostatic MD works well for small nanoplasmas, where the dipole approximation and the neglect of field propagation are justified. PIC codes average over the fine-grained atomic structure and thus neglect collisions and plasma microfields which is only justified at relativistic intensities or in weakly coupled plasmas and makes the treatment of large plasma volumes possible. We introduce a novel microscopic particle-in-cell (MicPIC) method that overcomes the above limitations with a P<sup>3</sup>M-type force decomposition. In MicPIC, long-range electromagnetic interactions are described on a PIC level, on which particles are represented by wide Gaussian distributions on a relatively coarse numerical grid. When two particles come close, the PIC field is replaced by the analytic electrostatic field to resolve microscopic (Mic) interactions. As a first application, we study the resonant excitation of metal-like clusters (Mie plasmon and laser in resonance) where we found plasma waves in surprisingly small clusters at moderate laser intensities ( $< 10^{14} \,\mathrm{W/cm}^2$ ). A detailed analysis of the wave dynamics and its impact on absorption and ionization will be presented.

### P II.31

# Interaction of ultrarelativistic electron and proton bunches with dense plasmas

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For the first time it was proposed to employ the nonrelativistic electron bunches propagating through plasma for generation of high plasma wakefields [1]. High-energy bunch electrons generate the wake plasma wave (wake) in such a way that the energy from a bunch of electrons is transferred to the plasma wave through Cherenkov resonance radiation producing high electric fields (wakefields). Later, it was shown that the relativistic electron bunches can generate plasma waves with high relativistic phase velocity including the transverse electromagnetic waves efficiently radiated out of plasma [2]. The idea to accelerate the charged particles in a plasma medium using collective plasma fields belongs to G. I. Budker, V. I. Veksler and Ia. B. Fainberg [3]. For a detailed review about the modern status of this research field we would like to refer a reader to [4]. Recently, the possibility of generation of high power wakefields

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(proton-bunch-driven plasma-wakefield acceleration) of terra-watt amplitude using the ultrarelativistic proton bunches was introduced [5]. In the present work this idea along with the employment of ultrarelativistic electron bunch is discussed at the qualitative level. We solve the analytical problem of interaction of ultrarelativistic electron and proton bunches with plasma [6]. These bunches remain relativistic in the frame of reference of generated by these bunches wakes compared to those considered earlier which were nonrelativistic [7]. Namely, we make an estimation of plasma parameters, maximum amplitude of the generated wakefield when the ultrarelativistic electron and proton bunches are employed and plasma, bunch lengths at which the maximum amplitude of the wakefield can be gained.

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### P II.32

## Computer simulation of energetic charged particles formation in laser plasmas

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Results of experimental investigation of energetic ions production in laser plasmas (in addition to [1]) are compared with theoretical calculations, which were carried out by using radiative MHD model [2], as well as by numerical solution of Fokker-Plank equation under calculations of energy specters of ions and electrons in plasmas with strong electric and magnetic fields. Then computer simulation of high energy ions penetration through different filters (Al, Cu) in dielectric track detectors (CR-39, micafor ion energy measurement) and in tissue (for modeling processes of ray-therapy) had been produced by using mathematical models [3].

This work was supported by DAAD.

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## Ultra fast processes and evolution of structures of electric and magnetic fields in laser plasmas

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Results of experimental investigations and computer simulations (by using radiative MHD model ZEVS-2D [1]) of ultra fast processes in laser-produced plasmas are represented. We considered different conditions of laser beams -target systems (in vacuum and in gases: air, hydrogen, argon - under different pressures), for picosecond laser beams (from Nd YAG-laser) with maximum intensities in ranges I =60 TW/cm<sup>2</sup>-600 PW/cm<sup>2</sup> and for different metallic targets (Ta, Al and etc.). The structures of strong electric and magnetic fields are varied with time due to hydrodynamics and development of explosive instabilities in current caring plasmas of laser-produced discharges. The "droplets" of dense plasmas with freezing strong magnetic fields were investigated by using Faraday-rotation method in parallel with interferometric measurements of plasma densities with high spatial and time resolutions. The acceleration of ions in strong fields leads to intensive bombard of metallic targets and hence to its nuclear activation. The effect of induced radioactivity after pulse-periodic interaction of intensive laser radiation with metallic targets is considered too (in addition to [2]).

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#### P II.34

## Effect of relativistic and ponderomotive nonlinearities on second harmonic generation

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In the present paper, the authors have investigated the effect of self-focusing on Second harmonic generation (SHG), when both the relativistic and ponderomotive nonlinearities are operative. Due to combined effect of relativistic and ponderomotive nonlinearities, electrons are expelled from the high field region to the low field region by a ponderomotive force whereas ions are not expelled due to their inertia, the nonlinearity in the dielectric constant of the plasma comes by electron mass variation due to laser intensities and due to changes in electron density on account of the ponderomotive force. On account of this redistribution, transverse density gradient is established in the plasma which in turn generates a plasma wave at the pump frequency. This plasma wave further interacts with the incident laser beam and a second harmonic is

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generated. Combined effect of relativistic and ponderomotive nonlinearities on second harmonic yield is analyzed and results are compared with the case when only relativistic non-linearity is operative.

### **Dusty plasmas**

#### P II.35

# Influence of polarization phenomena on radial distribution function of dusty particles

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A pseudopotential model of intergrain interaction in dusty plasmas is proposed to take into account both the electrostatic polarization and the screening phenomena. The derivation is entirely based on the renormalization theory of plasma particles interaction developed in [1]. The dusty particles are supposed to be conductive such that the polarization phenomenon can strictly be treated in the charge image approximation. Such an assumption imposes no restraint of generality on the consideration because the polarization effects are essential for accurate description of intergrain interaction potential. The pseudopotential model is then used in the hypernetted chain approximation for the dust component to obtain the radial distribution function which reveals the non-monotonic behavior at sufficiently large values of the coupling parameter. This can be viewed upon as a short- or even long-range order formation in the dusty component of the plasma. This work is a fundamental extension of [3] where the similar procedure was utilized to describe the interaction of all plasma components. It has to be mention here that in the Yukawa potential is a limiting case of the proposed pseudopotential model of intergrain interaction.

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### Electrodynamic confinement of dust particle at atmospheric conditions

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Usually electrostatic fields created by electrodes of the trap are used for dust particle confinement in plasma devices. In this work the possibility of the dust particle confinement by alternating electric fields is investigated for improved quadrupole traps at atmospheric conditions. We are using numerical simulations to investigate the possibility of the forming of the dust structures in dynamic electrical traps such as the Paul trap or quadrupole trap. Numerical simulations of dust particles behaviour for forces acting on dust particles is considered, the influence of gas medium is taken into account by viscosity and random forces. In considered model the dust particle motion is described by the Langevin equation. Results of our simulations for Paul trap showed the appearance of standing waves of the dust particle density arising due to the dynamic effects of periodic electrical field of low frequency. The dependences of electric field amplitude and frequency needed for levitation of dust particles in a quadrupole trap have also been studied. The dependence of the equilibrium position of dust structures in a quadrupole trap versus the frequency of the alternating electric field is investigated. Our experimental results for quadrupole traps agree well with conclusions of mathematical simulations.

#### P II.37

### Thermodynamical properties of finite two-dimensional dust clusters

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A finite number of dust clusters confined in a two-dimensional electrostatic confinement are investigated. Numerical simulation is performed for dust ensemble of constant charge and in the presence of charge fluctuation when the dominant charging process is by particles collection. We focus on the heat capacity at constant volume. The temperature at which the heat capacity is maximal dependence on the screening parameter of inter-particle interaction. The effect of the eccentricity of confinement potential is also studied.

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## Structural and transport properties of dust formations in plasma gas mixtures in RF discharge

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Data from experiments in DC discharge reveal that the properties of dust formations change considerably if small heavy component is introduced [1-3] in a background gas. Possible mechanism of such behavior bases on a drift of heavy ions in a background of lighter component. Such drift leads to damping of ion heating in electric field and, if electric field reaches critical value, to consequent formation of supersonic ion jets [4]. This is characteristic for DC discharge where dust formations are confined in electric field of static strata. Investigation of structural and transport properties of dust formation in RF discharge of binary mixtures may also show interesting effects. In addition, it can also have some practical value as many scientific and practical applications of dusty plasma are characterized by binary or multi-component gaseous environment. In some applications fraction of second component rises due to accompanying processes of both chemical and physical nature. Present paper reports on experimental investigation of structural and transport properties of dust formations in a mixture of noble gases in RF capacitive discharge. In high frequency electric field dust formation is relatively easy dragged by ion flow. Therefore, physical processes in discharge have strong impact on dust formation and can be studied from the observation of its properties.

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#### P II.39

## Clusters of diamagnetic dust particles in a cusp magnetic trap under microgravity conditions

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At the last conference PNP-13 we presented a new approach to the formation of macroscopic Coulomb clusters [1-3]. It is based on the known possibility of the levitation of diamagnetic bodies in a nonuniform steady-state magnetic field. We have experimentally and theoretically demonstrated principal possibility of the formation of Coulomb clusters in a magnetic trap. However, in the terrestrial laboratory setup in magnetic

fields ~1 T we have obtained only small clusters containing a few particles. And our next step is the investigation of rather extended three-dimensional Coulomb clusters under conditions of microgravity. First experiments on the formation of Coulomb clusters containing about 103 graphite particles under microgravity conditions have been performed aboard the International Space Station [4]. In these experiments Coulomb clusters are confined in a cusp magnetic trap generated by a specially designed setup. In this contribution we present results of the MD simulation of the formation of Coulomb clusters in the cusp magnetic trap and their behavior under conditions of the experiment [4]. We have numerically calculated the distribution of magnetic field in the cusp trap at different values of the currents in electromagnet coils created the field. Using the distribution we have simulated the excitation of cluster oscillations by changing the currents in the coils and their damping. The MD simulation yields the size and shape of the dust cluster similar to the observed ones in [4] and the oscillation parameters closed to experimental data.

This study was supported by the program for basic research of the Presidium of the Russian Academy of Sciences "Matter at high energy densities" and by the RFBR Projects 10-02-01428, 10-02-90056 and 11-02-01051.

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#### P II.40

# On the diffusion and oscillations of the dust particles in the gas discharge plasma

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Dusty plasma is the plasma which contains solid particles of the size far larger then the size of atoms. Dusty plasma is often found in nature, especially in astrophysical objects such as planetary rings, comet tails, etc. So, the study of the fundamental properties of dusty plasmas is of a particular importance. The method of the Langevin dynamics found its recent wide application in studies of the dusty plasma properties [1-5]. In work [6] the results of investigation of the velocity autocorrelation functions (VAF) and diffusion of dust particles were described. Now we present the results of the continuation of work [6], ones of them are the spectral intensity of VAF and the oscillation frequencies, which were obtained on the basis of this spectral intensity. The dependences of oscillation frequencies on the dusty plasma parameters were investigated. The analysis of obtained results and conclusions were made.

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### Shielding of the dust particle charge in a nonequilibrium plasma

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In the present paper the influence of non-locality of the electron energy distribution function on dust particle potential is considered in two-component plasma of noble gases and nitrogen at atmospheric pressure. The plasma is generated by an external gas ionization source, the ionization rate was changed in the range  $10^{12}$ - $10^{17}$  cm<sup>-3</sup>s<sup>-1</sup>. The point sink model was chosen for analytical and numerical calculations, where the electron and ion absorption by microparticle were taken into account. EEDF non-locality effects were included by the additional energy balance equation, which binds the local value of the electron mean energy with the plasma parameters in neighbor points.

#### P II.42

### Selection effect of dust particles by size and form factor

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The effect of selection of the dust granules exists in the process of self-organizing of dusty subsystem in complex plasmas. In the presented paper the new technique of quantitative studying of this effect is offered. Particles having arbitrary form and wide distribution of the sizes were used in experiments. It was found that particles with the different sizes and the form in volume dust structures are selected in depending on conditions of a dusty plasma trap. In the case of intensive ionization (in striations in the glow discharge) particles with the maximal of the specific charge were selected. In contrast, in the case of weakly ionization (in dead volume chambers) particles with the smallest specific charge were present in structures.

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### Plasma-dust system in the surface layer of the illuminated part of the moon

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A renaissance is currently being observed in investigations of the Moon, which are planned in the People's Republic of China, United States, India, and European Union. The Luna-Glob and Luna-Resourse missions (the latter jointly with India) are being prepared in Russia. Future investigations of dust near the surface of the Moon are important. For these investigations, it is planned to equip the Luna-Glob and Luna-Resourse stations with instruments both for direct detection of dust particles over the surface of the Moon and for optical measurements. The day-side surface of the Moon is charged under the action of the electromagnetic radiation of the Sun, solar wind plasma, and plasma of the Earth's magnetotail. The day-side surface of the Moon interacting with solar radiation emits electrons owing to the photoelectric effect, which leads to the formation of the photoelectron layer over the surface. Dust particles located on or near the surface of the Moon absorb photoelectrons, photons of solar radiation, electrons and ions of the solar wind, and, if the Moon is in the Earth's magnetotail, electrons and ions of the magnetospheric plasma. All these processes lead to the charging of dust particles, their interaction with the charged surface of the Moon, and rise and motion of dust. Small dust particles (smaller than several microns), repulsing from the surface, can rise from several meters to kilometers over the surface of the Moon. Thus, dust over the Moon is a component of the dusty plasma system. Investigations of this system in the surface layer of the Moon are of significant interest, including technological interest, for instruments mounted on lunar stations, choice of a Moon landing site, etc. Here, we consider the motion of single charged dust particles, we study the dusty plasma system in the surface layer of the Moon. The situations where a dust particle is formed over lunar regolith regions and hydrogen enriched regions of the surface of the Moon are analyzed. The problem of the existence of the dead zone near a lunar latitude of 80°, where, as was assumed earlier, dust particles cannot rise over the surface of the Moon, is discussed. The dust density over the surface of the Moon is calculated.

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# Motion of a projectile penetrating a dust crystal under microgravity

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Subsonic motion of a large particle moving through the bulk of a dust crystal formed by negatively charged small particles is investigated using the PK-3 Plus laboratory onboard the International Space Station. Tracing the particle trajectories show that the large particle moves almost freely through the bulk of plasma crystal, while dust particles move along characteristic  $\alpha$ -shaped pathways near the large particle. In the hydrodynamic approximation, we develop a theory of nonviscous dust particles motion about a large particle and calculate particle trajectories. A good agreement with experiment validates our approach.

#### P II.45

# Plasma crystals and liquids in experiments on the Interanional Space Station

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The short review of results for investigating the dusty plasma physics under microgravity conditions with the help of the unique facilities "Plasma Crystal-3" and "Plasma Crystal-3Plus" is presented. The possibility to study phenomena in strongly-coupled three-dimensional dusty-plasma system at the kinetic level has been demonstrated. In the case of an action of an external low frequency electric field in the dusty plasma the structural phase transition from an isotropic system to electrorheological plasma that is identical to electrorheological liquid has been observed. The data on the liquid-crystal transition in the large, three dimensional dusty-plasma system, consisting of more than a million highly charged dust particles are presented.

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## The diagnostics of dusty plasma parameters on the basis of the microscopic properties

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In this paper the method for determination of dusty plasma parameters are proposed on the basis of the dependence between microscopic and macroscopic properties of the system. The microscopic properties such as pair correlation functions, velocity autocorrelations functions, static structure factors were experimentally obtained by DC and RF gas discharges. In order to determine the plasma parameters the sum rules and normalization relations were used. The present results are compared with data from other methods. Obtained results can be applied for creation of new diagnostic methods for determination of plasma parameters.

#### P II.47

# Spectroscopic diagnostics of plasma gas mixtures in radio frequency discharge

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In the present work optical spectral diagnostics of buffer and dusty plasmas was carried out. For comparison of the spectra we used plasmas of different gases: argon plasma, argon-hydrogen mixture and the mixture of argon and methane gases. Methods of optical diagnostics of plasma have obtained the great development and play important role in the investigation of the plasma properties. They permit to obtain extensive information on the plasma parameters (the temperature, the number density of plasma particles, etc.) and to achieve a more detailed understanding of physical processes in the system. In contrast to traditional diagnostic methods, optical diagnostics is not contact and allows us to define different physical parameters of the plasma without affecting it. The experimental setup was described in detail in previous work [1]. The main element of the experimental setup is the two parallel plates of the RF reactor. The upper electrode is grounded. The lower electrode is capacitively coupled to the RF generator, which has frequency 13.56 MHz. Both electrodes are 19 cm in diameter with a spacing of 2 cm. Energy contribution under the experimental conditions was 0.02 W/cm<sup>3</sup>. At beginning of the experiment the chamber is properly pumped. As a working medium the mixtures of gases (Ar, H<sub>2</sub>+Ar, CH<sub>4</sub>+Ar) were used, and the pressure of working gas was varied in region 0.05-2.00 Torr. In experiments polydisperse dust particles of Al<sub>2</sub>O<sub>3</sub> with an average radius of 4 microns were used. We have observed that in all obtained spectra the dominant lines are the lines of argon atoms in the range of 700-900 nm; that causes reddish glow of plasma. In experiments the

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significant increase in the lines intensities of argon was observed in the argon-hydrogen mixture in comparison with spectra of pure argon and argon-methane mixture. One possible explanation for such phenomenon can be a resonant energy transfer from the hydrogen molecules to hydrogen atoms, which occupy the metastable excited level (2s), and then excite the argon atoms. On the basis of obtained spectra we also determined the temperature and number density of electrons for different values of pressure and power of discharge.

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#### P II.48

### Correlated motion of macroparticles in ordered dusty structure

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Results of experimental investigation of correlations between macroparticle displacements in ordered structures of complex (dusty) plasma are presented. To obtain data of spatial macroparticle positions in the structure for the observation time video acquisition and processing system is carried out to capture video, to extract still images and process their. To compare behavior two macroparticles displacing relative to its initial positions correlation coefficient is used. For macroparticles forming ordered structures in plasma of a dc glow discharge degree of correlation for the different pair of macroparticles is varied, and the smaller displacement period the stronger correlations but for all that it doesn't depend on physical conditions (the gas pressure and the current density).

#### P II.49

# Phase transitions in spherical dust clusters: Analysis using the triple correlation function

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While strongly correlated plasmas usually exist at low temperature or very high pressure, in dusty plasmas these effects are accessible at room temperature. Dust particles usually accumulate high negative charge inside a plasma which is responsible for their strong repulsive interaction and high coupling. When confined in a parabolic trap, these particles form spherical clusters with a characteristic shell structure.

In recent years the phase transition-like crossover from a crystal to a liquid-like state

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has attracted high interest, e.g. [1]. While the radial melting is now well understood, here we concentrate on the loss of intra-shell order.

To this end we apply the Triple Correlation Function for which we sample, for all pairs of particles, both radial coordinates and the angle between the directions from the trap center to the particle [2,3]. This quantity resolves both correlation within one shell and angular correlations between different shells.

The analysis of angular correlations in the outer shell of Coulomb clusters reveals a striking similarity with the properties of extended two dimensional systems including indications for Kosterlitz-Thouless behavior.

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#### P II.50

# "Temperature" concept at description of dust particles dynamics in gas discharge

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Dust particles in gas-discharge plasma achieve high kinetic energy, which exceeds both own temperature of dust particle material and temperatures of ions and electrons under certain conditions. Dust particles oscillate along the vertical and horizontal axes differently under certain conditions. The mechanism of energy transfer from discharge to dust particles motion is divided into several parts. Warming up of dust particles vertical oscillations is considered separately from the heating of horizontal oscillation, as these processes are determined by several different phenomena due to near-electrode layer anisotropy. The mechanism of energy transfer from vertical to horizontal oscillations of dust particles is based on parametric resonance. The outflow of energy from the dust particles oscillations due to friction on the neutral gas is also taken into account. These steps of scheme of energy transfer have different characteristic and relaxation times.

Features of mechanism of energy transfer between vertical and horizontal oscillations allow us to divide the concept of temperature for two subsystems of vertical and horizontal oscillations. Reasons for using the concept of temperature for description of dust particles dynamics are discussed. The proximity of velocity distribution to Maxwell distribution is one of the main factors, which allows us to use the concept of temperature for such systems. Consideration of dust particles horizontal and vertical velocity distribution and mechanism of energy transfer between these subsystems reveals the possibility of two different kinetic temperatures of dust particles. Molecular dynamics method was used to verify the theoretical calculations.

## The structure factor and critical point of weakly ionized dense dusty plasma systems

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In simple liquids the existence of two distinct fluid phases, gas-liquid transition and critical point require the presence of an attractive well in the pair interaction potential [1]. In dense dust clouds, the self-field of any test grain is not completely screened until it reaches its neighboring grains and hence dust collective effects become important. Moreover, ion neutral collisions and mostly the source of plasma particles (necessary to compensate for their absorption on dust) play an important role on the shape of the potential distribution around a dust particle.

In order to define a proper pair effective interaction potential the complex plasma system can be considered as a one-component gas of "dressed" dust particles with the background plasma medium providing screening, charging and dissipation. The plasma fluxes maintaining the grain equilibrium charge become collective and result in the existence of an attractive well in the effective dust-dust interaction potential [2], in a wide range of parameters that are accessible to experiments [3].

This form of the potential can be used to solve the Ornstein-Zernicke equation in the mean spherical approximation for dust particles [4]. This approach provides the analytical expressions for the direct correlation function of the dust particles C(r), the structure factor S(k) and the excess energy in terms of free parameters.

At first, a long range attraction in the pair potential of interaction produces a minor pre-peak in the structure factor at long wavelengths, appearing before the main peak due to the nearest neighbors [5]. Strong resolution in such wavelength regions will experimentally verify collective attraction and can indirectly be used for the determination of the ion distribution in the vicinity of the grain (which is defined with the help of an unspecified parameter in order to account for absorption on dust and non-linear effects like trapped ions and potential barriers). Moreover, the equation of state can be found from the long wavelength limit of the structure factor S(0), allowing to find the critical region and the coexistence of the two fluid phases by plotting the isotherms and also the critical temperature and density by the inflection point of the curves [6].

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# Study of the dust-free region near an electric probe in dusty plasma

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Last years phenomena in the region near probe in dusty plasmas are intensively studied. So, motion of the individual dust particle in the ion sheath around Langmuir probe was investigated in work [1,2], which showed a significant affect of the ion drag force on the particles trajectory [2]. In this paper we consider the behavior of the large number of dust particles in the region around the electric probe with a negative potential. The size of the dust-free region, which depends on the probe potential, was determined by the visual observation in experimental setup. The comparative analysis of the results obtained at the different conditions of the discharge was made. At rising of the pressure in the discharge tube the size of the dust-free region increases. Visual measurements of the dust-free region radius can be used to determine the basic parameters of the background plasma without measuring of the traditional current-voltage characteristics, and will be useful to explain the formation of layers of charged particles around the probe.

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#### P II.53

# Diagnostics of parameters of plasma in near-electrode area of RF-discharge under condition of dust monolayer

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Parameters of plasma in near-electrode layer of rf-discharge are investigated experimentally in conditions of levitation of dust monolayer. We consider a new method of diagnostics of plasma parameters: mean electric field, ion density and ion velocity. Also we estimate screening parameter and a value of particle charge. A criteria of stable levitation of dust monolayer is presented. New experimental data concerned with stable levitation of dust monolayer in plasma of near-electrode layer of rf-discharge. A comparison with the existing theoretical and numerical data as well as with results obtained by independent methods of diagnostics is presented.

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### Glow discharge positive column with dust particles in neon

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Experimental and numerical study of positive column of glow discharge in neon was motivated by the need to understand and simulate the changes of plasma parameters induced by micron size particles, introduced into the discharge tube.

Experiments were carried out at pressure of 0.35 torr in a cylindrical discharge tube of 16.5 mm i.d. with two ring electrodes, glued into the tube walls in front of the region of formation of dust structure for measuring the voltage drop in the positive column. Dust structures were formed from mono disperse 2.55  $\mu m$  melamine formaldehyde dust particles. The registration of images of dust structures was carried out, the corresponding current-voltage characteristics of discharge and the same characteristics of free discharge without dust particles were measured. Dust particles caused additional electron losses on their surface and changed plasma ionization balance that required the increase of electric field strength to maintain the discharge current. The highest increase of the electric field strength was registered in the presence of large-scale dust structures containing a large number of dust particles and also for spatially stable structures. Such structures were observed at currents of 0.5 – 1 mA.

The simulation was based on the model of the uniform glow discharge positive column with dust particles, used previously in air [1]. In this study, the model considers formation and diffusion of electrons, ions and metastable neon atoms, which play important role in ionization of neon. The electron temperature, transport coefficients and reaction rate coefficients for electron impact reactions with finite energy threshold were obtained using the SIGLO Database [2] and the electron Boltzmann equation solver BOLSIG+ [3]. For description of dust particle charging the OML approximation was applied. The quenching of metastable atoms within the dust cloud is also considered. The numerical task was solved at discharge parameters where the most stable dust structures were observed.

In simulations, the dust particle distribution was given by axially symmetrical flat profile with slight end blurring. The increment of the electric field strength in presence of dust structures reflecting the influence of dust particles on the plasma of glow discharge was measured and simulated.

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- [3] Hagelaar G.J.M. and Pitchford L.C., 2005, Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models, Plasma Sources Sci. Technol., 14, 722 doi:10.1088/0963-0252/14/4/011

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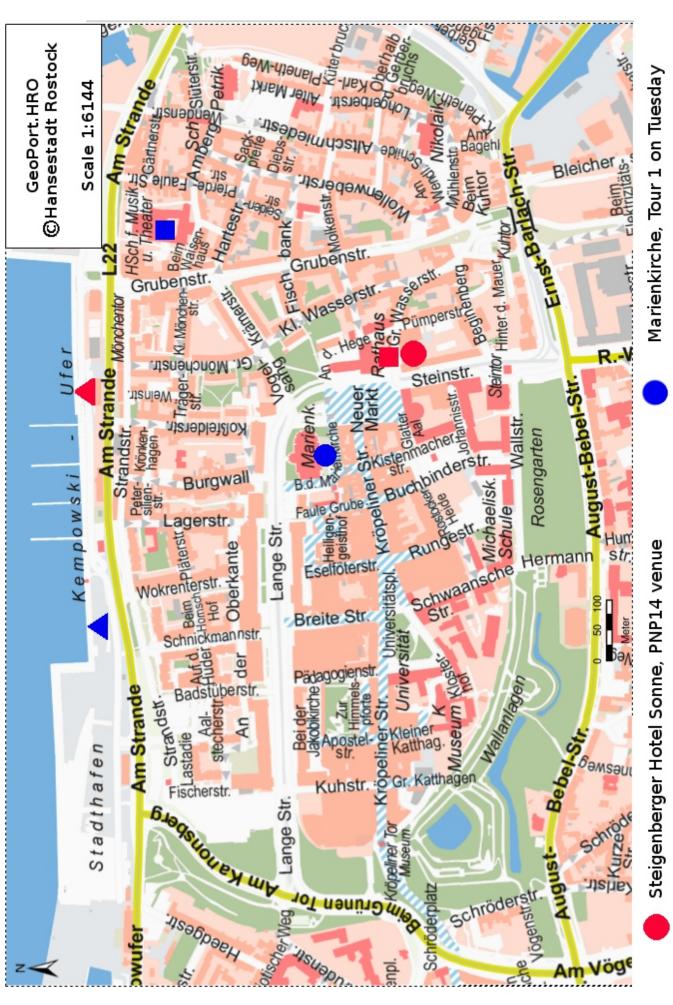
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### Notes



University for Music and Theater, Concert on Monday

Start boat trip on Wednesday

"Lokschuppen", Conference Dinner on Thursday

Town Hall, Poster Sessions on Tuesday

and Thursday evening

### **PNP-14 Program**

### Rostock, September 9-14, 2012

### Steigenberger Hotel Sonne, Neuer Markt 2, 18055 Rostock, Tel. (+49) 381-4973-0

Time- table	Sun Sep 09	Mon Sep 10	Tue Sep 11	Wed Sep 12	Thu Sep 13	Fri Sep 14	
08:45		Opening					
09:00		I1 Knudson	I5 Glenzer	I9 Keitel	I11 Killian	T42 Tahir	09:00
09:30		T1 Ternovoi	T13 Fletcher	T25 Liseykina	T31 Ott	T43 Deutsch	09:20
09:50		T2 Dai	T14 Hamel	T26 Andreev	T32 Kalman	T44 Hazak	09:40
10:10		T3 Benage	T15 Mintsev	T27 Kull	T33 Mulser	T45 Schram	10:00
10:30 – 11:00				Coffee Break			10:20 - 10:50
11:00		I2 Ceperley	I6 Fortney	I10 Goree	I12 Zhang	T46 Fennel	10:50
11:30	<del></del>	T4 Desjarlais	T16 Nettelmann	T28 Petrov	T34 Trickey	T47 Winkel	11:10
11:50	Arrival	T5 Lorenzen	T17 Potekhin	T29 Starostin	T35 Morozov	T48 Moll	11:30
12:10	₹	T6 Dufty	T18 Gryaznov	T30 Kopnin	T36 Ramazanov	T49 Raitza	11:50
			_			Closing	12:10
12:30 – 14:00		Lunch & Discussions			Lunch & Discussions		
14:00		I3 Fortov	I7 Falcone		I13 Ng		
14:30		T7 Clerouin	T19 Döppner		T37 Ludwig		
14:50		T8 Recoules	T20 Tschentscher		T38 Collins		
15:10		T9 Ziaja-Motyka	T21 Rosmej	Buses leave on	T39 Norman		
15:30 – 16:00	oby (	Coffee Break		13:00 at Hotel Sonne (lunch	Coffee Break		
16:00	Lok ne)	I4 Koenig	18 Gericke	bags provided):  Excursion to	I14 Sano		
16:30	on (	T10 Mazevet	T22 Sperling	Hansestadt	T40 Yoneda	Departure	
16:50	atic el s	T11 Gamaly	T23 Rozmus	Stralsund -	T41 Krainov		
17:10	jisti Hot	T12 Matsuda	T24 Tkachenko	"Ozeaneum" and			
17:30	Registration (Lobby Hotel Sonne)	HEDgeHOB Collaboration	Poster Session I (Town Hall)	Old Town	Poster Session II (Town Hall)		
18:30	ne Lobby nne)	Board Meeting	(Town Hall)				
19:30	Welcome Reception (Lobby Hotel Sonne)	Concert: University for	Tour 1: Astronomical Clock Marienkirche		Conference Dinner:		
20:30	Wel Receptic Hotel	Music and Theater (HMT)	Tour 2: Night walk through Old Town		"Lokschuppen" (City Harbour)		

All sessions are held in room Apollo I-III (ground floor) of Steigenberger Hotel Sonne.
Invited Talks (I): 30 minutes, Topical Talks (T): 20 minutes including discussions.
Poster sessions are held in the Town Hall (lobby) – two minutes walking distance.
The PNP business meeting (Program Committee) is scheduled on Tue Sep 11 during the lunch break.
Lunches and coffee will be served in the lobby of Hotel Sonne (free for all participants).
WLAN is available in rooms Apollo I-III during the conference (free for all participants).







