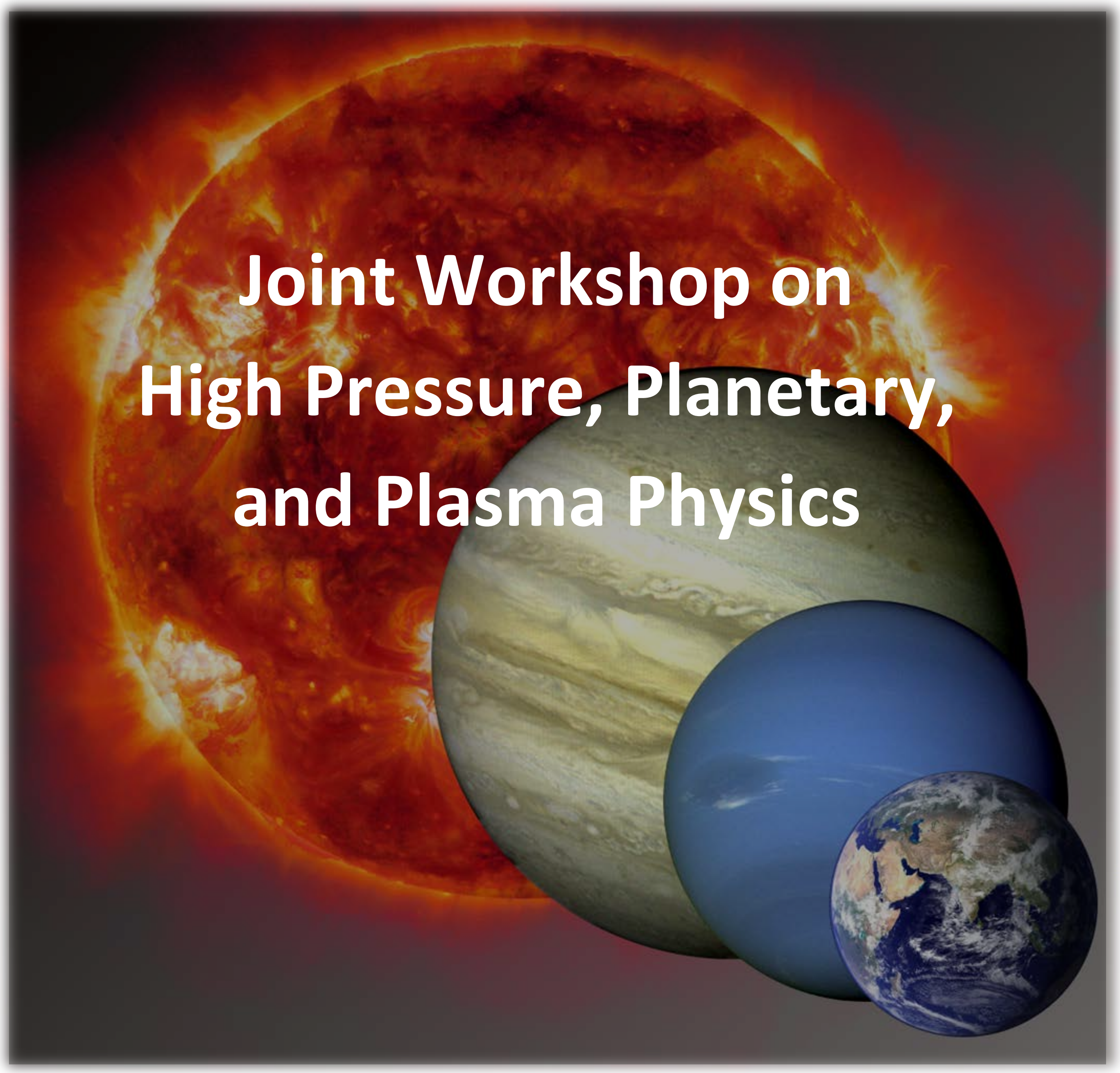

DLR Berlin-Adlershof
Institute of Planetary Research
October, 23rd – 25th, 2013

DLR
Deutsches Zentrum
für Luft- und Raumfahrt e.V.
in der Helmholtz-Gemeinschaft

Joint Workshop on High Pressure, Planetary, and Plasma Physics
October 23 – 25, 2013
DLR, Institute of Planetary Research, Berlin, Rutherfordstraße 2
Meeting Room: Rotunde

The main objective of this workshop is to bring together scientists from different fields of expertise to discuss topics related to extreme planetary environments in terms of high temperature and high pressure. This meeting is also intended to inspire new projects and offer scientific opportunities for future collaboration between workshop participants from distinct research fields.

Group picture taken in front of the main entrance of DLR Berlin

Meeting website for more information, registration, abstract submission, and logistical details:

http://indico.desy.de/conferenceDisplay.py?ovw=True&confId=8221

SOC: Frank Sohl, Hanns-Peter Liermann, Ronald Redmer, Gerd Steinle-Neumann, Thomas Tschentscher, Frank W. Wagner.

LOC: Matthias Kreuzeder (DESY), Laura Brumm, Ana-Catalina Plesa, Tina Rückriemen, Frank W. Wagner, Frank Sohl.

Image Credit Front Cover: NASA/JPL/RPIF/DLR

Day 1, Wednesday October 23

12:00	**Registration**	
12:15	**Light Lunch**	
13:15	**Opening**	T. Spohn/F. Sohl

Session 1	**New Perspectives for High Pressure Physics**	*page 8*
13:30	Shock physics and hypervelocity impact events (invited)	Kai Wünnemann
14:00	The workings of rocky planet interiors	Tilman Spohn
14:25	Warm dense matter and the interior of giant planets	Ronald Redmer
14:50	New perspectives for matter under extreme states research: the high energy density instrument at the European XFEL	Thomas Tschentscher
15:15	Discussion	
15:30	**Coffee**	

Session 2	**Structure of Matter I**	*page 13*
16:00	Plate tectonics and mantle convection in super-Earths (invited)	Paul Tackley
16:30	The phase diagram of MgO	Daniel Cebulla
16:50	Elastic and inelastic properties under simulated Earth's mantle conditions in large volume apparatus in conjunction with synchrotron radiation	Hans J. Müller
17:10	Finite strain elasticity and planetary impacts	Detlef de Niem
17:30	**End of Session**	

17:30 Session 9 Poster Reception (Technisches Kabinett) *page 41*

Constraints against a porous CI chondritic Ceres	Wladimir Neumann
Thermal and compositional evolution of the Martian mantle	Thomas Ruedas
Formation of stable geochemical reservoirs: Implications for the thermo-chemical evolution of Mars	Ana-Catalina Plesa
Se and S partitioning between silicate and metallic melts using at conditions of the Earth's core formation using laser heated DACs and SR-µXRF	Manuela Borchert
Key characteristics of the iron snow regime in planetary cores	Tina Rückriemen
High-pressure phase diagram of carbon	Manuel Schöttler
Ab initio simulations for the structure factor of liquid and warm dense aluminum	Hannes Rüter
Calculation of the structure factor with ab initio simulations for warm dense matter	Kai-Uwe Plagemann
Monte Carlo simulations of ionization potential depression in dense plasmas	Michal Stransky
H-He demixing and evolution of Saturn	Robert Püstow
Determinability of the Love number k_2 of exoplanets from transit timing variations	Szilard Csizmadia
Investigation of plasma jet creation and collimation mechanisms	Alexander Pelka
Current status and future plans for the Extreme Conditions Beamline (ECB), P02.2, PETRA III, DESY	Hanns-Peter Liermann

20:00 End of Session

Day 2, Thursday October 24

Session 3	**Rocky Planet Interiors**		*page 17*
09:00	Influence of variable thermodynamic parameters on mantle dynamics (invited)	Nicola Tosi	
09:30	Mantle rheology, internal dynamics and tidal heating of massive rocky exoplanets	Frank Wagner	
09:50	High values of thermal conductivity for Fe in planetary cores: the puzzle pieces and what they mean for planetary dynamos	Gerd Steinle-Neumann	
10:10	Implications of silicon in Mercury's core on geodesy measurements	Attilio Rivoldini	
10:30	**Coffee**		

Session 4	**Structure of Matter II**		*page 22*
11:00	Thomson scattering at FEL’s and planetary interiors (invited)	Gianluca Gregori	
11:30	Single pulse laser heating in double-stage diamond anvil cell: Probing material under planetary interior conditions	Zuzana Konopkova	
11:50	Investigation of phase transitions of iron under extreme dynamic compression with XANES measurements at LCLS	Marion Harmand	
12:10	Planetary physics research program at Facility for Antiprotons and Ion Research (FAIR) at Darmstadt: the LAPLAS experiment	Naeem Tahir	
12:30	**Lunch Break**		

Session 5	**Giant Planet Interiors**	*page 26*
14:00	The outer planets in the Solar system (invited)	Ravit Helled
14:30	Magnetic field generation and interior dynamics of Jupiter and Saturn	Johannes Wicht
14:50	Water-ammonia mixtures at high pressures	Mandy Bethkenhagen
15:10	Investigating phase transition kinetics of planetary bodies using the dynamic diamond anvil cell at the European XFEL	Emma McBride
15:30	**Coffee**	

Session 6	**Facilities, Instruments, and Diagnostics**	*page 30*
16:00	Ab initio equation of states for planetary and exoplanetary modeling (invited)	Stephane Mazevet
16:30	Equation of state measurements of CH plastic at Gbar pressures using the National Ignition Facility	Tilo Döppner
16:55	High-pressure research at the high-energy density instrument at the European XFEL	Karen Appel
17:15	Opportunities for laboratory astro- and planetary physics at the matter-in-extreme-conditions end station at LCLS	Bob Nagler
17:40	Announcements	
17:45	**End of Session**	

19:30 Workshop Dinner, Restaurant "Lehmofen", Freiheit 12, 12555 Berlin-Köpenick

Day 3, Friday October 25

Session 7	**Melting and Crystallization**	*page 34*
09:00	Minerals and melts at extreme conditions: Insights from molecular simulations (invited)	Sandro Jahn
09:30	Crystallization of a deep magma ocean and its consequence for planetary thermal evolution	Doris Breuer
09:50	Ice and salt crystallization in supercooled aqueous solutions: Requirements concerning thermophysical parameters	Olaf Hellmuth
10:10	Subsurface water oceans on icy Solar system bodies	Frank Sohl
10:30	**Coffee**	

Session 8	**Atmospheres and Origins**	*page 38*
11:00	Exploring atmospheres of hot mini-Neptunes and extrasolar giant planets orbiting different stars (invited)	Yamila Miguel
11:30	Modeling brown dwarfs using ab initio equation of state data	Andreas Becker
11:50	Planetary climate and the link to planetary interiors	Philip von Paris
12:10	Observational constraints on the critical core mass from the rocky exoplanet population	Heike Rauer
12:30	**Closeout and Adjourn**	

12:30 Light Lunch

Session 1
New Perspectives for High Pressure Physics

Chairs: Ravit Helled and Frank Sohl

1.1	Shock physics and hypervelocity impact events (invited)	Kai Wünnemann
1.2	The workings of rocky planet interiors	Tilman Spohn
1.3	Warm dense matter and the interior of giant planets	Ronald Redmer
1.4	New perspectives for matter under extreme states research: the high energy density instrument at the European XFEL	Thomas Tschentscher

1.1: **Shock physics and hypervelocity impact events**

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Cratered landscapes on planetary surfaces testify to the frequency of hypervelocity impacts suggesting the general importance of collision events in the evolution of all bodies in the solar system. The hypervelocity nature of such collision events implies the generation of strong shock waves at pressures in excess of several hundreds of GPa causing vaporisation and melting of rocks after release from shock pressure. The vast majority of the kinetic energy of the impactor is transferred to the target in terms of internal energy that is distributed by the propagation of shock waves deep into the target body heating up its interior.

The extreme pressure/temperature conditions during such events strongly depend on the velocity at impact and material properties that are difficult, often impossible, to simulate in laboratory experiments. Numerical models can overcome the laboratory limitations in terms of the size-scale and extreme thermodynamic conditions; however, accurate equations of state that require detailed characterization of materials by laboratory shock wave experiments are crucial for a quantitative analysis of the shock-induced consequences of hypervelocity impact events.

We present results from numerical modelling of the propagation of impact-induced shock waves on the scale of small grains of mineral phases and open pore space [1,2] to planetary-sized collision events [3,4,5] and compare our results with laboratory experiments. In particular we investigated the effects of material properties [6,7] on the propagation of shock waves and quantify the shock-induced heating of matter as a consequence of meteorite impact.

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1.2: **The workings of rocky planets**

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The interiors of rocky planets can be considered as heat engines in complex systems that convert thermal energy into other energy forms such as gravitational, magnetic field, and deformational energy. The thermal and chemical evolutions of these bodies are mainly driven by solid-state convection in the interiors, involving a wide range of different time scales.

Structural models of rocky planet interiors are usually chemically layered in mantles and cores, including high-pressure ice layers if icy satellites are considered. The successful construction of chemically layered interior structure models of planetary bodies invokes the knowledge of thermodynamic state variables, petrology and geochemistry of planetary materials, equation-of-state parameters for the local density, compaction of porous materials, thermal and electrical material properties, intrinsic energy sources, chemical reactions, and pressure-induced phase transformations [1,2]. The mantle viscosity is strongly dependent on temperature, pressure, and the bulk volatile content of rocky planets. For super-Earths, probably the most critical consideration is how the mantle viscosity would vary with pressure and thus with depth. It is possible that increasing pressure will frustrate deep mantle convection, reducing the vigor of mantle convection. Possibly, the generation of a magnetic field in a putative iron-rich core will be impossible, if super-Earths at all have earth-like cores [3].

On active planets like the Earth, deep volatile cycles and exchange processes between geochemical reservoirs are invoked with plate tectonics. Thermal evolution models accounting for partial melt production and degassing suggest that the transition from the stagnant to the plate-tectonic like, mobile lid regime of a planet could be a function of total mass and bulk composition [4]. Furthermore, an abiotic world is found to have a much drier mantle than the present Earth but may have a similar surface coverage by continents. Through the effect of water on the mantle rheology, the biotic world would tend to be tectonically more active and have a more rapid long-term carbon-silicate cycle [5].

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1.3: **Warm dense matter and the interior of giant planets**

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The behavior of warm dense matter (pressures up to several TPa, temperatures of several eV) is of paramount importance for interior models of giant planets such as Jupiter and Saturn. However, the high-pressure phase diagram of even the simplest and most abundant elements hydrogen and helium is not well known. For instance, metal-insulator transitions and demixing may occur at high pressures which would strongly affect the interior and magnetic field structure of giant planets. At present, ab initio molecular dynamics simulations based on finite-temperature density functional theory are able to determine the equation of state, the high-pressure phase diagram, and the transport properties with high accuracy for a wide range of densities and temperatures as relevant for solar and extrasolar giant planets [1,2]. Most interestingly, new predictions for the location of a first-order liquid-liquid phase transition in dense hydrogen and the demixing region in H-He mixtures have been given recently. New results were also derived for molecular systems (e.g. water [3] and ammonia [4]) and minerals (e.g. MgO [5], Fe alloys [6]) at high pressures which are important for icy (Uranus, Neptune) and rocky planets (Earth, Super Earths).

While experiments with diamond anvil cells and state-of-the-art shock-waves (driven by gas guns, high explosives, lasers, pulsed power) are limited to several Mbar, heavy ion beams (FAIR Darmstadt) and X-ray free electron lasers (LCLS Stanford and the future European XFEL Hamburg) provide so far unprecedented possibilities to probe materials up to several TPa. Novel diagnostic tools such as X-ray Thomson scattering, X-ray absorption near-edge spectroscopy or proton radiography have to be applied for this purpose. Experiments at these (and other) new high-pressure platforms and the rapidly increasing computational power and success of ab initio simulations will lead to a much better understanding of matter under extreme conditions and thereby of the structure, evolution and formation of planets in our solar system and around other stars.

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1.4: **New perspectives for matter under extreme states research: the high-energy density instrument at the European XFEL**

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Free-electron laser facilities provide new applications in the field of dynamic high-pressure research. The European X-ray Free Electron Laser (XFEL) [1] will start user operation in 2016 and will provide photon energies of up to 25 keV. With a photon flux of ca 10^{12} photons/pulse, a pulse duration of 2 – 100 fs and a repetition rate of up to 4.5 MHz, this facility will provide unique opportunities to study fast processes such as dynamic compression in solids.

The high-energy density instrument (HED) [2] is one of the six baseline experiments at the European XFEL and now has entered the technical design phase. For this instrument, it is planned to integrate several high performance lasers to be used in pump-probe type experiments. A high-energy nanosecond pulse duration laser system will enable studies of materials at extremely high pressures. Ramp-compression by nanosecond shaped laser pulses will extend the range of high-pressure conditions accessible at hard X-ray sources up to 10 Mbar at comparatively low temperatures. A suitable optical laser system with repetition rates of 0.1 and 10 Hz was recently proposed by an international consortium. In addition to this system also laser for ultrahigh intensities of close to 10^{20} W/cm^2, again operating at 0.1 to 10 Hz repetition rate, and a ultrashort pulse system with down to 15 fs pulse duration and mJ pulse energies at MHz repetition rates matching the X-ray delivery will be provided at the HED instrument. Probing of the laser generated excited states will be performed with the high energy X-ray free electron laser (FEL). In the energy range between 5 and 25 keV, it will be possible to study samples by X-ray diffraction, X-ray spectroscopy and imaging techniques. Due to the high excitation energies, diffraction patterns will have excellent quality and a wide range of elements (Z > 22) will be accessible by X-ray absorption spectroscopy. The high intensity and time structure will enable time-resolved studies of the samples generated during dynamic compression. In addition, the high brilliance and coherence of the FEL radiation will enable spatially resolved studies.

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Session 2
Structure of Matter I

Chairs: Nicola Tosi and Ana-Catalina Plesa

2.1	Plate tectonics and mantle convection in super-Earths (invited)	Paul Tackley
2.2	The phase diagram of MgO	Daniel Cebulla
2.3	Elastic and inelastic properties under simulated Earth's mantle conditions in large volume apparatus in conjunction with synchrotron radiation	Hans J. Müller
2.4	Finite strain elasticity and planetary impacts	Detlef de Niem

2.1: **Plate tectonics and mantle convection in super-Earths**

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Convection of the rocky mantle is the key process that drives the evolution of the interior: it causes plate tectonics, controls heat loss from the metallic core (which generates the magnetic field) and drives long-term volatile cycling between the atmosphere/ocean and interior. It is commonly thought that plate tectonics is necessary for planetary habitability because of its role in long-term volatile cycles that regulate the surface environment, yet exactly how plate tectonics arises is still quite uncertain; other terrestrial planets like Venus and Mars instead have a stagnant lithosphere. Nevertheless, simple scalings [1] as well as more complex models [2] indicate that plate tectonics should be easier on larger planets (super-Earths), other things being equal. Recent models find that compositional heterogeneity in the lithosphere plays an important role in facilitating plate tectonics [3,4]. The mode of plate tectonics may have changed with time on Earth and other planets as they cool. Chemical differentiation caused by partial melting plays an important role in mantle and core evolution [5,6]. Deep mantle dynamics is strongly influenced by the physical properties of rock changing greatly with pressure, and this will have much more so in super-Earths. We have used density-function theory to calculate the rheology of the post-perovskite phase to pressure of 1 TPa, and used this in simulations of super-Earth mantle and plate dynamics. Although a large viscosity increase is predicted along an adiabat, the deep mantle is found to adopt a super-adiabatic temperature profile such that its viscosity does not become extremely high and it still convects to lose heat. If, as is likely, large terrestrial planets started off molten then it is likely that their deep interiors are still very hot and active.

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2.2: **The phase diagram of MgO**

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A large number of Super Earths, i.e. planets in the mass range 1-10 Earth masses, 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 than in the interior of the Earth due to their greater mass.

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

Using ab initio molecular dynamic simulations (VASP [3]), we have determined the phase diagram for MgO up to 20,000 K and 800 GPa. In particular, the transition from the solid to the molten salt phase has been studied using diffusion analyses and pair distribution functions. The transition from the NaCl- (B1) to the CsCl- (B2) structure in solid MgO is determined by calculating the respective free enthalpies. Here the free energy was determined by integration of the internal energy in addition to computations in the harmonic approximation with the PHONOPY code [4].

With the resulting simulation data the phase diagram of MgO is constructed and the equation of state (EOS) is calculated. The electrical conductivity and the reflectivity are determined along the Hugoniot curve in order to compare to experimental data [5]. The B1-to-B2 and the liquid-solid transition line are checked against earlier simulation and experimental results.

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2.3: **Elastic and inelastic properties under simulated Earth's mantle conditions in large volume apparatus in conjunction with synchrotron radiation**

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The interpretation of highly resolved seismic data from Earth's deep interior require measurements of the physical properties of Earth's materials under experimental simulated Earth's mantle conditions. More than a decade ago seismic tomography clearly showed subduction of crustal material can reach the core mantle boundary under specific circumstances. That means there is no longer space for the assumption deep mantle rocks might be much less complex than deep crustal rocks known from exhumation processes. Considering this geophysical high pressure research is faced the challenge to increase pressure and sample volume at the same time to be able to perform in situ experiments with representative complex samples. High performance multi anvil devices using novel materials are the most promising technique for this exciting task. Recent large volume presses provide sample volumes 3 to 7 orders of magnitude bigger than in diamond anvil cells far beyond transition zone conditions.

The sample size of several cubic millimeters allows elastic wave frequencies in the low to medium MHz range. Together with the small and even adjustable temperature gradients over the whole sample this technique makes anisotropy and grain boundary effects in complex systems accessible for elastic and inelastic properties measurements in principle. The measurements of both elastic wave velocities have also no limits for opaque and encapsulated samples. The application of triple-mode transducers and the data transfer function technique for the ultrasonic interferometry reduces the time for saving the data during the experiment to about a minute or less. That makes real transient measurements under non-equilibrium conditions possible. A further benefit is, both elastic wave velocities are measured exactly simultaneously. Ultrasonic interferometry necessarily requires in situ sample deformation measurement by X-radiography. Time-resolved X-radiography makes in situ falling sphere viscosimetry and even the measurement of elastic and inelastic properties in the seismic frequency range achievable. This way current geophysical high pressure research is more and more bridging the gap between indoor and outdoor seismology.

2.4**: Finite Strain Elasticity and Planetary Impact**

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Early planetary evolution is characterized by giant impacts occurring for an extended period of time, sufficient for planetary differentiation, the formation of a core and lithosphere. Continuum mechanical models of such catastrophic events still assume the validity of linear elasticity for the deviatoric part of stress. In contrast, there is no doubt that the high-pressure equation of state (EOS) is non-linear. The assumption of linear elasticity is questionable, at least 'when worlds collide' or when rotational breakup of a fast-spinning body is regarded. Here a comprehensive description is derived where the EOS generating both the pressure and deviatoric stress corresponds to finite strain, or large-deformation theory of elasticity. A numerical method has been implemented in an Eulerian multi-material hydrocode. Simulation examples are given. Further questions dealt with are: Is the hyperelastic EOS used to generate the deviatoric stress arbitrary, or is there a universal form? How to describe finite-deformation plasticity, which numerical methods are useful? Are there observable differences to linear elasticity, accessible in high-velocity laboratory experiments?

Session 3
Rocky Planet Interiors

Chairs: Johannes Wicht and Doris Breuer

3.1	Influence of variable thermodynamic parameters on mantle dynamics (invited)	Nicola Tosi
3.2	Mantle rheology, internal dynamics and tidal heating of massive rocky exoplanets	Frank Wagner
3.3	High values of thermal conductivity for Fe in planetary cores: the puzzle pieces and what they mean for planetary dynamos	Gerd Steinle-Neumann
3.4	Implications of silicon in Mercury's core on geodesy measurements	Attilio Rivoldini

3.1: **Influence of variable thermodynamic parameters on mantle dynamics**

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The coefficients of thermal expansion and thermal conduction control the way heat is transported in the interior of solid planets by advection and diffusion, thereby affecting the dynamics and thermal evolution of the mantle. Although it is well known that both parameters exhibit significant variations with pressure and temperature, most simulations of mantle convection still assume them to be constant. We collected data of thermal expansivity from a database of first-principles calculations [1], and of thermal conductivity from experimental studies [2,3] and derived simple analytical parametrizations for the major upper- and lower-mantle phases [4]. By using these parametrizations in numerical models of mantle convection, we show that the large-scale dynamics of the mantle is strongly affected by the pressure and temperature dependence of these two parameters. On the one hand, this indicates that the variability of the thermal expansivity and conductivity should be routinely taken into account in geodynamic simulations. On the other hand, it confirms the importance of experimental and theoretical efforts devoted to the accurate determination of these parameters at high pressure and temperature.

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3.2: **Mantle rheology, internal dynamics and tidal heating of massive rocky exoplanets**

WAGNER, Frank (DLR, Institute of Planetary Research) frank.wagner@dlr.de

The pressure dependence of mantle rheology is often not taken into account when dealing with rocky exoplanet interiors due to limited knowledge about the rheological properties of silicate perovskite and post-perovskite at a high degree of compression [1]. In this talk, I will use the Kepler-36b exoplanet [2] as a case study to examine the rheological and thermal structure inside of massive rocky planets. Particular emphasis will be placed on addressing the question of how the present thermal structure and tidal heating rates are affected by a mantle rheology dominated by silicate post-perovskite. I will show that the mantle viscosity depends weakly on planetary mass owing to a viscosity-temperature feedback mechanism (e.g., [3], [4]). Furthermore, a super-adiabatic temperature gradient in the deep interior ([3], [5]) implies substantially higher core and mantle temperatures than previously reported from parameterized convection models (e.g., [6]). This has implications for the possible existence of a self-sustained magnetic field in rocky exoplanets that will be discussed. I will also discuss how tidal dissipation rates of rocky exoplanets are affected by the obtained rheological structure by calculating body tide potential Love numbers for different visco-elastic rheological models.

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3.3: **High values of thermal conductivity for Fe in planetary cores: the puzzle pieces and what they mean for planetary dynamos**

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The electronic transport properties of liquid metals at high pressures are critical to understanding processes associated with the thermal evolution of planets and magnetic field generation in the liquid portion of their cores. Terrestrial planets, such as the Earth, contain iron as the primary core elements. Unfortunately, the understanding of electronic (σ) and thermal conductivity (κ) from experiments relies on extrapolations both in temperature and pressure and a number of scaling relations, which include: (1) σ~1/T, (2) σ constant along (and across) the melting line, (3) and the validity of the Wiedemann-Franz law [e.g., 1]. Ab-initio simulations based on density functional theory provide an alternative route to both σ and κ of liquid metals at high pressure and temperatures and allow testing of the relations outlined above as well as address contradicting results from shock wave experiments for σ of Fe [2,3]. Using such methods we have recently computed the electric transport properties of Fe and some of its alloys [4] at high temperature and pressure. For all systems investigated we find that the σ~1/T relation is violated, and that electrical conductivity at conditions of the Earth's core is higher by a factor of three than previously thought, in agreement with subsequent computations [5] and experiments [6]. With the Wiedemann-Franz law holding approximately κ of liquid Fe and its alloys is also considerably higher than in previous models, which requires a reconsideration of the thermal state and evolution of the Earth's core. Here we present the evidence and inherent assumptions that lead to the high conductivity values and review dynamic consequences for geodynamics.

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3.4: **Implications of silicon in Mercury's core on geodesy measurements.**

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The measurements of the gravitational field of Mercury by MESSENGER and improved measurements of the spin state of Mercury provide important constraints on the interior structure of Mercury. In particular, these data give strong constraints on the radius and density of Mercury's core and on the core's concentration of sulfur if sulfur is the only light element in the core. Although sulfur is ubiquitously invoked as being the principal candidate light element in terrestrial planet's cores its abundance in the core depends on the redox conditions during planetary formation. MESSENGER data from remote sensing of Mercury's surface indicate a high abundance of sulfur and confirm the low abundance in FeO supporting the hypotheses that Mercury formed under reducing conditions. Therefore, substantial amounts of other light elements like for instance silicon could be present together with sulfur inside Mercury's core. In this study we build interior structure models with both silicon and sulfur in the core that agree with the measured 88 day libration amplitude and polar moment of inertia of Mercury and calculate their tides.

Session 4
Structure of Matter II

Chairs: Paul Neumayer and Tilo Döppner

4.1	Thomson scattering at FEL's and planetary interiors (invited)	Gianluca Gregori
4.2	Single pulse laser heating in double-stage diamond anvil cell: Probing material under planetary interior conditions	Zuzana Konopkova
4.3	Investigation of phase transitions of iron under extreme dynamic compression with XANES measurements at LCLS	Marion Harmand
4.4	Planetary physics research program at Facility for Antiprotons and Ion Research (FAIR) at Darmstadt: the LAPLAS experiment	Naeem Tahir

4.1: **Thomson scattering at FEL's and planetary interiors**

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The high-pressure transitions into phases with temperature above 5,000 K and densities above 1 g/cm^3 are poorly understood. This warm dense matter regime is expected to exist in liquid form in the interiors of giant planets and many white dwarf stars. Here, we report results of experiments creating extreme conditions similar to those found in the envelope of white dwarfs using the combination of an optical and x-ray laser. Scattered x-rays reveal a highly correlated state, where the electrostatic energy significantly exceeds the thermal energy of the ions. Strong Coulomb forces are expected to induce the formation of a crystalline ion structure, but no evidence of a phase transition is observed. We will present new experimental and computational results of the dynamic structure factors and related thermodynamic properties of such plasmas.

4.2: **Single-pulse Laser Heating in Double-Stage Diamond Anvil Cell: Probing material under planetary interior conditions**

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With the new high-brilliance x-ray source, the European x-ray free electron laser (EXFEL), coming online in 2016, new possibilities of investigating matter at conditions approaching warm dense matter state are emerging. It is anticipated that this new technology will help us in furthering our knowledge of the conditions matter exists in interiors of planets which will impact our understanding of the planetary composition and structure and also planetary history.

The main focus is to determine crystal structure and chemical composition of materials (solids possibly perhaps melts) under previously unattainable pressure-temperature conditions using static compression technique. Pressure will be generated in a modified diamond anvil cell equipped with secondary small diamond anvils or nanodiamonds semi-spheres capable of reaching up to 8 Mbar. Further developments of this technique are currently being pursued [1]. Simultaneously, pulse-laser heating with microsecond pulse duration will be utilized to reach temperatures of 2,000-10,000 K. The sample under P-T conditions achieved by the double-stage DAC and laser pulses will be probed by short (a hundred of femtoseconds) and intense x-ray pulses of the EXFEL train. Due to the short time scale inherent to these experiments, it is anticipated that all the experimental information is collected within one shot (~ a microsecond).

This approach will complement laser driven compression and it will be unique in the conditions off adiabats and isentropes. It would open a large P-T space that is not accessible by shock-wave and ramp compression techniques.

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4.3: **Investigation of phase transitions of iron under extreme dynamic compression with XANES measurements at LCLS**

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An accurate knowledge of the properties of iron alloys at high pressures and temperatures is crucial for geophysics and planetary science. In particular, detailed information on melting curves and solid phases are required to anchor the Earth's thermal profile at the Inner-Outer Core Boundary (IOCB) and to assess the solid or liquid nature of exoplanet cores. In that context, X- ray FEL sources coupled with high-energy lasers are affording unique opportunities to measure microscopic structural properties at extreme conditions.

Here we present a recent study devoted to investigate the solid-liquid transition in laser-shocked iron using X-ray Absorption Near-Edge Spectroscopy (XANES). The experiment was performed at the MEC end-station of the LCLS facility at SLAC in Stanford. In parallel, a detailed theoretical study based on ab-initio calculations has been performed and will be presented against experimental measurements.

4.4: **Planetary physics research program at Facility for Antiprotons and Ion Research (FAIR) at Darmstadt: the LAPLAS experiment**

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High intensity, strongly bunched and well-focused beams of energetic heavy ions have emerged as a novel, very efficient tool for generating High Energy Density (HED) matter including Warm Dense Matter (WDM) and strongly coupled plasmas, in the laboratory. **F**acility for **A**ntiprotons and **I**on **R**esearch (**FAIR**) at Darmstadt has already entered into construction phase that includes building of a huge heavy ion synchrotron, SIS100 (100 Tm magnetic rigidity) that will deliver high intensity beams of all stable particle species from protons up to uranium. HED physics research is an important part of the FAIR research program. Since the heaviest particles (uranium) deposit the highest amount of specific power in the target material, mostly, the HED research will be done using a uranium beam. According to the design parameters, the SIS100 is expected to generate a uranium beam having an intensity of 5×10^{11} ions delivered in a 50 ns long bunch. A wide range of particle energy (400 MeV/u – 2.7 GeV/u) will be available while the beam can be focused to a circular spot with a radius of around 1 mm. Provisions have also been made to generate a hollow beam with an annular focal spot to perform cylindrical compression experiments. These beam parameters lead to a specific power deposition of 15 TW/g in solid lead which will allow one to access those parts of the HED matter phase diagram that have never been accessed before.

It is important to note that ion beams provide unparalleled flexibility as they can be used to generate HED matter not only by isochoric heating but also by shock compression. Over the past decade, extensive theoretical work that is based on sophisticated 2D and 3D numerical simulations and analytic modeling, has been done to design different HED physics experiments for the FAIR. This work has resulted in a nice and very wide range scientific program named, **HEDgeHOB** (**H**igh **E**nergy **D**ensity matter **g**enerated by **H**eavy I**O**n **B**eams). This program includes several HED physics experiments that are suitable to study for example, Equation-of-State of HED matter [1], planetary physics [2,3], hydrodynamic instabilities [4,5] and others. Work is in progress to design more experiments in other areas of HED physics. In this talk we present details of the planetary physics research program at FAIR employing the **LAPLAS** [**LA**boratory **PLA**netary **S**cience] experimental scheme.

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Session 5
Giant Planet Interiors

Chairs: Yamila Miguel and Ronald Redmer

5.1	The outer planets in the Solar system (invited)	Ravit Helled
5.2	Magnetic field generation and interior dynamics of Jupiter and Saturn	Johannes Wicht
5.3	Water-ammonia mixtures at high pressures	Mandy Bethkenhagen
5.4	Investigating phase transition kinetics of planetary bodies using the dynamic diamond anvil cell at the European XFEL	Emma McBride

5.1: **The Outer Planets in the Solar System**

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Jupiter and Saturn, the gas giants, have large masses and are composed mostly of hydrogen and helium with a smaller fraction of heavy elements. Uranus and Neptune, the ice giants, consist mainly of rocks/ices with thin gaseous hydrogen/helium envelopes. The compositions and internal structures of the planets in the outer solar system are derived from structure (interior) models which use the measured physical properties of the planets such as mass, gravitational coefficients J_{2n}, equatorial/mean radius, 1 bar temperature, rotation rate, and occasionally, the atmospheric composition. Interior models, however, are typically static 1D models, and therefore do not account for the continuous planetary shape, dynamical contributions (i.e. winds) and magnetic field generation.

In this talk I will briefly describe how planetary interiors are modeled, and will present interior models of the four outer planets in the Solar System. New results, the importance of EOSs, uncertainties and open questions, and future investigations will be presented. Finally, I will briefly discuss how the internal structure and composition of the planets reveal valuable information on their formation history.

5.2: **Magnetic field generation and interior dynamics of Jupiter and Saturn**

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The surface dynamics of Jupiter and Saturn is dominated by a banded system of fierce zonal winds. The depth of these winds remains unclear but they are thought to be confined to the very outer envelopes where hydrogen remains molecular and the electrical conductivity is small. The dynamo responsible for the dipole dominated magnetic fields of both gas giants, on the other hand, likely operates in the deeper interior where hydrogen assumes a metallic state. Here we present numerical simulations that attempt to model both the zonal winds and the interior dynamo action in an integrated approach. Using the anelastic version of the MHD code MagIC we explore the effects of density stratification and radial electrical conductivity variations. Based on ab-initio results, the electrical conductivity is assumed to remain constant in the thicker inner metallic region and decays exponentially towards the outer boundary throughout the molecular envelope. Our results show that the combination of stronger density stratification and a weaker conducting outer layer is essential for reconciling dipole dominated dynamo action and a fierce equatorial zonal jet. Previous simulations with homogeneous electrical conductivity show that both are merely exclusive with solutions either having strong zonal winds and multipolar magnetic fields or weak zonal winds and dipole dominated magnetic fields. The particular setup explored here allows the equatorial jet to remain confined to the weaker conducting region where is does not interfere with the deeper seated dynamo action. This is not an option for the additional mid to higher latitude jets observed on Jupiter and Saturn. Our results suggest that their depth should be limited to the outer weaker conducting region to enable dipole dominated dynamo action. Since all jets tend to be geostrophic in our simulations, however, they reach right through the convective shell. Dipole dominated dynamo action is thus only possible for particularly weak mid to high latitude jets.

5.3: **Water-ammonia mixtures at high pressures**

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The interior of the Giant Planets Uranus and Neptune contains large amounts of water, ammonia and methane (referred to as ”planetary ices”). Many observable properties of these planets, such as luminosity, gravitational moments and magnetic fields, are thought to be determined by the physical and chemical properties of matter within this ice layer.

Hence, the phase diagrams, equations of state and structural properties of these materials and their respective mixtures are of great interest.

We present equation of state data for water-ammonia mixtures at pressures up to several Mbar and in the temperature range from 500 K to 10,000 K obtained by ab initio simulations based on density functional theory using the VASP code [1]. Furthermore, we investigate the impact of the complex chemistry on the fluid properties as well as exotic phases forming at these high pressures. In particular we discuss superionic phases, which have been predicted for the pure compounds water [2,3] and ammonia [2,4]. These superionic phases are characterized by highly mobile hydrogen ions in a lattice of oxygen and nitrogen ions, respectively, and might be present in the mixture as well.

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5.4: Investigating Phase Transition Kinetics of Planetary Bodies using the Dynamic Diamond Anvil Cell at the European XFEL

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Low-Z molecular solids such as H_2, N_2 and methane are the primary constituents of planetary bodies such as the Jovian planets. In order to better understand planetary interiors, a comprehensive understanding of the phase transition kinetics of these materials is required. Furthermore, to construct accurate models of such planetary bodies, knowledge of the equations-of-state and phase diagrams of these materials is needed.

For decades the diamond anvil cell (DAC) has been an indispensable tool in the investigation of matter at extreme conditions. However, experiments aiming to provide structural information on low-Z molecular systems are limited for a variety of reasons, including the failure of the diamond anvils at ~300 GPa, in addition to the exceedingly small sample sizes of poor X-ray scattering materials at such pressures. Furthermore, traditional DACs do not allow the precise control of compression rates required to investigate phase transition kinetics – phase transition kinetics have primarily been investigated using shock compression techniques that inherently suffers from a large increase of sample temperature causing the sample to reach a point in P-T space far from the planetary isentrope.

An alternative technique to investigate such systems is the dynamic diamond anvil cell (dDAC), a novel device developed by members of our team to achieve tunable and rapid compression rates [1]. Increasing pressure very rapidly (500 GPa/µs) provides an avenue for reaching pressures in excess of 400 GPa. In such rapid compression cycles, the sample experiences extreme pressures for only a very short time of the order of µs. Within we are proposing to combine the dDAC with brilliance and time resolution of the European XFEL, operating at 24 keV at a repetition rate of 4.5 MHz. This will enable the collection of an entire equation-of-state in one compression experiment.

An experimental setup for a dDAC experiment at the European XFEL will be proposed, including the combination of this device with laser driven compression techniques [2,3] and heating/cryogenic cooling techniques to investigate an even larger volume of phase space.

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Session 6
Facilities, Instruments, and Diagnostics

Chairs: Sandro Jahn and Thomas Tschentscher

6.1	Ab initio equation of states for planetary and exoplanetary modeling (invited)	Stephane Mazevet
6.2	Equation of state measurements of CH plastic at Gbar pressures using the National Ignition Facility	Tilo Döppner
6.3	High-pressure research at the high-energy density instrument at the European XFEL	Karen Appel
6.4	Opportunities for laboratory astro- and planetary physics at the matter-in-extreme-conditions end station at LCLS	Bob Nagler

6.1: **Ab initio equation of states for planetary and exoplanetary modeling**

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Using ab initio molecular dynamics simulations, we recently calculated equation of states for five main constituents of planetary interiors: H, He, H_2O, SiO_2 and Fe. These equations of states are multi-phases, include liquid and solid phases, and aim at building planetary and exoplanetary interior models solely based on ab initio predictions. This talk will concentrate on the results obtained for silica and iron where we used ab initio predictions, laser shock experiments combined with XANES (X-ray near edge spectroscopy) measurements to study the physical properties of these constituents at planetary core conditions.

This work is supported in part by the French Agence National de la Recherche under contract PLANETLAB ANR-12-BS04-0015.

Further reading

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6.2: **Equation of state measurements of CH plastic at Gbar pressures using the National Ignition Facility**

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We have used the capabilities of the National Ignition Facility (NIF) to conduct absolute equation of state and opacity measurements of plastic CH along the principal Hugoniot at unprecedented pressures, approaching 1 Gbar. Such experiments are important to benchmark atomic physics models and improve simulations of indirectly-driven ICF implosions in which CH currently is the primary ablator material. A 5 ns long, 1.3 MJ laser pulse at 351 nm, generating a hohlraum drive with 290 eV peak radiation temperature, launches a strong shock wave into a 2.2 mm diameter plastic ball. The induced pressures by the spherical shock wave increase as the shock converges allowing to obtaining a range of Hugoniot states in a single experiment. Pressures reach ~ 1 Gbar as the shock wave coalesces at the center of the CH target. We measure the radiography contrast at the shock front with a powerful Zn He-alpha backlighter source to infer compression. The opacity along the Hugoniot is also deduced, which is essential in Gigabar experiments as it changes significantly from its initial value. We will present results of first experiments in which the shock speed and compression, obtained from radiographic analysis, gave absolute Hugoniot states from 120 - 700 Mbar, which is an order of magnitude greater than previously measured in CH [1]. The measured EOS locus was consistent with the previous measurements, and significantly stiffer than the theoretical EOS used for comparison. Our analysis also gave the variation of opacity along the Hugoniot, which showed a decrease of an order of magnitude, approximately as expected from atomic physics calculations.

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6.3: **High-pressure research at the high-energy density instrument at the European XFEL**

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The high-energy density instrument (HED) is one of the six baseline instruments at the European XFEL. Besides the use of the X-ray FEL beam as a possible pump and/or probe, it will be equipped with a high-energy, an ultra-high intensity and a high repetition rate optical laser system. The foreseen high-energy laser is a 100 J-class laser with a pulse duration of 1 -20 nanoseconds. The expected repetition rate is > 1Hz. In combination with the X-ray FEL beam as a probe, it will enable unique studies of condensed matter at extremely high pressures and at short time scales.

In this contribution, the X-ray instrumentation and foreseen X-ray techniques at HED will be presented as well as prototype experiments in the field of high-pressure research as proposed during a recent user consortium meeting for this instrument. These include dynamic compression and shock compression experiments as well as experiments of pre-compressed matter.

6.4: **Opportunities for Laboratory Astro- and Planetary Physics at the Matter in Extreme Conditions end-station at LCLS**

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Since the start of operation of the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory, many researchers have seen the potential of doing extraordinary research with its superior X-ray beam. Indeed, compared to standard synchrotron light sources, the brilliance of LCLS is ten orders of magnitude larger; the short (10s of femtosecond) highly intense (1-3mJ) pulses with photon energies ranging from 500 eV to 10 keV open up the study of materials under extreme condition of pressure, density and temperature. To optimally study such material, the Matter in Extreme Conditions (MEC) instrument was developed at LCLS. This instrument combines the superior LCLS beam with two high power laser systems, and diagnostics dedicated to the study of Warm Dense Matter, Hot Dense Matter and High Pressure and Density System. I will present the capabilities of the MEC instrument, and show some preliminary results of past experiment to show the potential MEC has to do experimental laboratory astrophysics and planetary physics experiments.

Session 7
Melting and Crystallization

Chairs: Gerd Steinle-Neumann and Frank W. Wagner

7.1	Minerals and melts at extreme conditions: Insights from molecular simulations (invited)	Sandro Jahn
7.2	Crystallization of a deep magma ocean and its consequence for planetary thermal evolution	Ana-Catalina Plesa
7.3	Ice and salt crystallization in supercooled aqueous solutions: Requirements concerning thermophysical parameters	Olaf Hellmuth
7.4	Subsurface water oceans on icy Solar system bodies	Frank Sohl

7.1: **Minerals and melts at extreme conditions: Insights from molecular simulations**

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Molecular modelling approaches have become a powerful tool to predict the structure, physical and thermodynamic properties of Earth and planetary materials under extreme conditions of pressure and temperature. The obtained properties serve as input parameters for large scale dynamic models and support the interpretation of experimental or field observations. In this talk, I will present new results of our recent activities in predicting high pressure crystal structures, mechanisms of related phase transitions as well as heat and material transport at extreme conditions.

7.2: **Crystallization of a deep magma ocean and its consequence for planetary thermal evolution**

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Early in the history of terrestrial planets, deep magma oceans may have formed as a consequence of large impacts. These magma oceans solidified during tens to hundred million years and the associated crystallization process plays a fundamental role for the subsequent evolution of these bodies. For Mars, the isotopic analysis of the so-called SNC meteorites suggests fractional crystallization to explain large scale chemical heterogeneities that may have been preserved over the entire planetary evolution [1,2]. The fractional crystallization leads to a chemical stratification characterized by a progressive enrichment in heavy elements from the core-mantle boundary to the surface. This results in an unstable configuration that causes the overturn of the mantle and the subsequent formation of a stable chemical layering.

To test this scenario, we investigated Mars' early thermo-chemical evolution using the code GAIA in a 2D cylindrical geometry [3] and assuming a detailed magma ocean crystallization sequence as obtained from geochemical modeling [1]. We used an initial composition profile adapted from [1], accounted for an exothermic phase transition between lower and upper mantle and assumed all radiogenic heat sources to be enriched during the freezing-phase of the magma ocean in the uppermost 50 km [2]. A stagnant lid forms rapidly because of the strong temperature dependence of the viscosity. This prevents the uppermost dense cumulates to sink, even when allowing for a plastic yielding mechanism. Below this dense stagnant lid, the mantle chemical gradient settles to a stable configuration. The convection pattern is dominated by small-scale structures, which are difficult to reconcile with the large-scale volcanic features observed over Mars' surface. Assuming that the stagnant lid will break, a stable density gradient is obtained, with the densest material and the entire amount of heat sources lying above the core-mantle-boundary. This leads to a strong overheating of the lowermost mantle, whose temperature increases to values that exceed the liquidus. Therefore, a fractionated global and deep magma ocean is difficult to reconcile with observations and leaves the question of the crystallization process open.

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7.3: **Ice and Salt Crystallization in Supercooled Aqueous Solutions: Requirements Concerning Thermophysical Parameters**

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Aerosol and hydrosol formation via multi-component vapour ↔ liquid ↔ solid phase transitions affect the chemical composition and radiative properties of the atmosphere, and may impact the exchange of energy and matter between the atmosphere, hydrosphere, biosphere, and geosphere. In the presentation, selected aspects of the microscopic description of salt and ice crystallisation in supercooled aqueous solution droplets and the required thermophysical parameters will be discussed. Our basic interest is to understand the catalytic effect of homogeneous salt crystallisation to stimulate heterogeneous freezing.

At first, an overview of the description of the growth/shrinking of a hygroscopic salt particle during hydration/dehydration in an atmosphere of a solvent vapour will be given. The approach allows the determination of (i) the actual size of the particle as a function of temperature and vapour saturation ratio, (ii) the threshold values of the vapour saturation ratio at the onset of complete salt dissolution (deliquescence) and salt crystallisation (efflorescence), and (iii) the chemical composition of the heterogeneous droplet.

Secondly, we outline the description of deliquescent/efflorescent-heterogeneous freezing of a supercooled solution droplet and briefly discuss the ‘closure problem’ in determining the nucleation rate, namely the estimation of the compatibility parameter at the contact line between the solution, an immersed therein freezing catalyser (a mixed soluble/insoluble core), and an ice embryo heterogeneously formed on the catalysing surface.

The aforementioned scenarios have been addressed as problems of atmospheric cloud research. The question to what extent these scenarios might also be relevant for the description of ice-ocean systems of icy moons in the Solar System or of comets cannot be answered and deserves, among others, detailed knowledge of the thermophysical constraints in such extreme environments. In the third part of the presentation we will outline some key features and deliveries of the "Thermodynamic Equation of Seawater 2010" (TEOS-10, http://www.teos-10.org/), developed by IAPWS/SCSW in cooperation with SCOR/IAPSO and endorsed as an international standard for oceanography by the UNESCO-IOC in 2009. The open-source code of TEOS-10 includes software implementations of this IAPWS formulation.

(Abbreviations will be explained in the presentation).

7.4: **Subsurface water oceans on icy solar system bodies**

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The state of knowledge about the structure and composition of the interiors of icy solar system bodies has been significantly extended by combining direct measurements from spacecraft, laboratory experiments, and theoretical modeling. The detection of induced magnetic fields in the vicinity of the Jovian satellites Europa, Ganymede, and Callisto was among the most surprising findings of the Galileo mission to Jupiter. The observed magnetic signature cannot be explained by solid ice and silicate rock. It rather suggests the existence of electrically conducting reservoirs of liquid water beneath the satellites' outermost icy shells that may contain even more water than all terrestrial oceans combined. The existence of these potentially habitable liquid water reservoirs on icy satellites is closely related to their internal structures, chemical compositions, and thermal states, and it is likely that subsurface water oceans even may have survived on smaller planetary bodies far from the Sun like, e.g., the Neptunian satellite Triton and large Kuiper belt objects beyond. The thermal state and geological activity of icy bodies are primarily dependent on the radiogenic heating of the rock component, additional contributions such as the dissipation of tidal energy, the efficiency of heat transfer to the surface, and the presence of substances that deplete the freezing point of liquid water. The temperature at which the ice melts will be significantly reduced by soluble substances like salts and/or incorporated volatiles such as methane and ammonia that are highly abundant in the outer solar system. Almost all outer solar system satellites are tidally locked and subject to time-variable radial and librational tides exerted by their primaries on the time-scale of their orbital period. The tide-induced internal redistribution of mass results in variations of surface gravity, tilt, stress and strain and corresponding measurements performed over several tidal cycles would provide important clues on the thickness and rheology of the outer ice shell and the density and composition of the ocean below. Furthermore, we will address the role that the low tidal strain rates could play in triggering processes, which might be even visible in the geological surface record of tidally locked icy bodies.

Session 8
Atmospheres and Origins

Chairs: Stephane Mazevet and John Lee Grenfell

8.1	Exploring atmospheres of hot mini-Neptunes and extrasolar giant planets orbiting different stars (invited)	Yamila Miguel
8.2	Modeling brown dwarfs using ab initio equation of state data	Andreas Becker
8.3	Planetary climate and the link to planetary interiors	Philip von Paris
8.4	Observational constraints on the critical core mass from the rocky exoplanet population	Heike Rauer

8.1: **Exploring atmospheres of hot mini-Neptunes and extrasolar giant planets orbiting different stars**

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Motivated by the diversity of exoplanets detected by ground and space surveys, we use a one-dimensional photochemical model that includes disequilibrium chemistry to build a grid of hot extrasolar giant and mini-Neptune atmospheres around F, G, K and M stars. We address the differences in hot exoplanet atmospheres according to the observables semi-major axis and stellar type, exploring their detectable atmospheric features. Many main sequence M stars present strong chromospheric activity that produces high-energy radiation. We particularly study the effect of this radiation in these hot exoplanet atmospheres. These planets are interesting targets for future observations, therefore, addressing their atmospheric structure and composition is a major issue and the aim of our work. Our atmospheric grid can be applied to current and future planetary observations to characterize exoplanet atmospheres and serves as a reference to interpret the results of atmospheric retrieval analysis.

8.2: **Modeling Brown Dwarfs using ab initio equation of state data**

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We present wide-range equations of state (EOS) for hydrogen and helium including accurate data derived from finite-temperature density functional theory molecular dynamics (DFT-MD) simulations for the warm dense matter regime using the VASP package [1]. This hydrogen/helium Rostock EOS (H/He-REOS) cover a wide range of temperatures and densities with a maximum error of 5% and reproduce data from high pressure experiments, for example the principal and precompressed Hugoniot curve and the 300 K isotherme derived from diamond anvil cell measurements, see [2].

Based on this ab initio data set we calculate interior models and mass-radius (MR) relations for Giant Planets and particularly for Brown Dwarfs. The latter need EOS data for the 1-bar level ($\rho \sim 10^{-5}$ g/cm^3, T$\sim$1000 K) as well as for central conditions with ~ 150 Gbar ($\rho \sim 250$ g/cm^3, T $\sim$ 3 MK). We compare our interior models and the MR relations with those based on the EOS of Saumon-Chabrier and van Horn (SCvH) [3].

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8.3: **Planetary climate and the link to planetary interior**

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Atmospheric pressure is unconstrained for terrestrial exoplanets but could vary over a wide range (consider e.g. Mars and Venus in the Solar System). It depends on a wide range of processes such as outgassing, escape and delivery. Atmospheric pressure will clearly influence habitabilty via e.g. the greenhouse effect, atmospheric scattering and (pressure-dependent) photochemistry.

In this work we will discuss the effects of varying atmospheric pressure upon habitabilty and biosignatures - in particular we will consider the link with outgassing and explore the question of the expected range of atmospheric pressures and compositions for rocky exoplanets given the constraints of current interior models.

8.4**: Observational Constraints on the Critical Core Mass from the Rocky Exoplanet Population**

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The number of exoplanets with measured radius, mass, and therefore mean density, is steadily increasing. Exoplanets provide us with a large sample of planets that we cannot obtain from our Solar System alone. Here, we discuss new insights to planet formation theories, which can be expected from an increasing statistics of well characterized exoplanets.

In particular, we discuss how this sample can be used to constrain the critical core mass for gas giant growth directly from observations of a large sample of close-in exoplanets and compare to state-of-the-art planet formation and evolution models. The present analysis suggests a critical core mass of 6 to 9 Earth masses to facilitate rapid accumulation of H-He envelopes. New ground- and space-based transit surveys targeting at planets around bright stars would considerably improve the exoplanet statistics in terms of mean densities for the corresponding low mass range [1].

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Session 9
Posters

Chairs: Frank W. Wagner and Tina Rückriemen

9.1	Constraints against a porous CI chondritic Ceres	Wladimir Neumann
9.2	Thermal and compositional evolution of the Martian mantle	Thomas Ruedas
9.3	Formation of stable geochemical reservoirs: Implications for the thermo-chemical evolution of Mars	Ana-Catalina Plesa
9.4	Se and S partitioning between silicate and metallic melts using at conditions of the Earth's core formation using laser heated DACs and SR-µXRF	Manuela Borchert
9.5	Key characteristics of the iron snow regime in planetary cores	Tina Rückriemen
9.6	High-pressure phase diagram of carbon	Manuel Schöttler
9.7	Ab initio simulations for the structure factor of liquid and warm dense aluminum	Hannes Rüter
9.8	Calculation of the structure factor with ab initio simulations for warm dense matter	Kai-Uwe Plagemann
9.9	Monte Carlo simulations of ionization potential depression in dense plasmas	Michal Stransky
9.10	H-He demixing and evolution of Saturn	Robert Püstow
9.11	Determinability of the Love number k_2 of exoplanets from transit timing variations	Szilard Csizmadia
9.12	Investigation of plasma jet creation and collimation mechanisms	Alexander Pelka
9.13	Current status and future plans for the Extreme Conditions Beamline (ECB), P02.2, PETRA III, DESY	Hanns-Peter Liermann

9.1: **Constraints against a porous CI chondritic Ceres**

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Considered as a protoplanet along with Pallas and Vesta[1,2], Ceres can be seen as one of the remaining examples of the intermediate stages of planetary accretion, which additionally is substantially different from most asteroids. Its low bulk density (2077±36 kg m^{-3}, see [3]) suggests a global ice mass fraction of ≈ 30% if the average porosity is negligible. Thermal models by [4] showed that Ceres has likely differentiated into a rocky core, an icy mantle and possibly a shallow still liquid layer above the core. Recent interior modelling by [5] has emphasized that warm surface temperature promotes the presence of a deep ocean in today's Ceres, provided sufficient fraction of ammonium and salts. Thereby, both studies assume an ice-silicate composition. Alternatively, Ceres could be made up of hydrated silicates (oxidised carbonaceous chondritic material) or be a homogeneous mixture of the CI chondritic material with significant porosity, without having a differentiated structure, as suggested by [6]. The observations by [3] and [7] of Ceres' shape are consistent with differentiation, but also allow for the structure suggested by [6]. Compaction of Ceres made up of hydrated silicates is estimated by [6] based on the compaction of sandstones at pressures ≥ 150 MPa, disregarding thereby the material specifications, such as the lower creep activation energy of hydrated silicates and the much higher effective pressure due to the porosity[8].

We have tested the possibility whether Ceres' low density can be explained with a porous interior, rather than with the presence of ice and show that the porous structure is rather unlikely. For a macroporosity of 10% and a CI chondritic composition, Ceres ultimately compacts due to hot pressing. From this consideration we conclude that it is rather unlikely that the low density of Ceres can be explained by a partially porous structure.

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9.2**: Thermal and compositional evolution of the martian mantle**

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We present numerical models for the thermochemical evolution of the mantle of Mars over the past 4 Gy. Specifically, we have developed a parameterized model of composition and thermoelastic properties of mantle material and combined it with the two-dimensional, anelastic, compressible convection and melting algorithm of STAGYY (e.g., Tackley, 1996) in a spherical annulus geometry (Hernlund & Tackley, 2008). These models include a detailed treatment of the effects of solid-solid phase transitions and of compositional changes that accompany generation and removal of mantle partial melt during magmatism, especially the redistribution of radionuclides and, in a subset of the models, water. The thermal evolution of the core is included as a parameterized one-dimensional model after Nimmo et al. (2004). Among other questions, we examine if a perovskite+ferropericlase layer exists at the base of the martian mantle, if long-lived plumes can explain the volcanic provinces, under which circumstances Mars may still be volcanically active, and how iron- and radionuclide-rich Mars is.

Results of the models are compared with geophysical and chemical observations from spacecraft and information from Martian meteorites. Most models yield crustal thicknesses between ~75 and 90 km, ancient depths for the Curie temperatures of candidate magnetic minerals that include the entire crust, and mechanical lithosphere thicknesses that increased from less than 100 km in the Noachian to ~200-250 km now. Generally, models with a large core, Mg#=0.75, and radionuclide contents based on those suggested by Wänke and Dreibus (1994) tend to explain observations best. However, only a subset of the models develops a pattern of mantle convection that evolves towards two or three large, long-lived plumes, and it takes at least ~2 Gy before this stage is reached. Moreover, the temporal stability of plumes decreases strongly if the influence of water on mantle viscosity is included, and models with a very low-viscosity deep mantle barely develop whole-mantle plumes at all. As Tharsis and probably Elysium are older than 2.5-3 Gy, model assumptions more complex than those made in this study are required to explain these major volcanic provinces.

Further reading

Ruedas, T.; Tackley, P. J.; Solomon, S. C. (2013): Phys. Earth Planet. Inter. 216, 32-58.

Ruedas, T.; Tackley, P. J.; Solomon, S. C. (2013): Phys. Earth Planet. Inter. 220, 50-72.

9.3**: Formation of stable geochemical reservoirs: Implications for the thermo-chemical evolution of Mars**

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The large variation in lithophile radiogenic isotope systems such as ^{87}Rb-^{86}Sr, ^{147,146}Sm-^{143,142}Nd, and ^{176}Lu-^{176}Hf obtained from the analysis of the SNC meteorites, infer the presence of three to four distinct chemical reservoirs that have been preserved over the entire thermochemical evolution of Mars [1].

We are running numerical models in a 2D cylindrical geometry to investigate the influence of chemical heterogeneities in Mars' mantle on the planet's thermochemical evolution. We present two scenarios (1) a fractional crystallized magma ocean as an initial condition, using the parameters from [2] and (2) partial melting and accounting for density variations due to mantle depletion. Both mechanisms lead to a chemical heterogeneous mantle. However, the magma ocean scenario is difficult to reconcile with other observations like late volcanic activity and crustal density [3, 4]. The alternative partial melting scenario does not present such difficulties. However, it remains to be clarified if this could explain the isotopic characteristic of the SNCs.

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9.4: Se and S partitioning between silicate and metallic melts using at conditions of the Earth's core formation using laser heated DACs and SR-µXRF

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The Earth's core mainly consists of a metallic Fe-Ni mixture. However, seismic observations show that the density is about 5-10% lower than expected for an Fe-Ni alloy under similar pressure and temperature conditions (e.g., [1,2]). This discovery initiated numerous studies to identify and quantify light elements in the Earth´s core. Among others, sulphur has been suggested to be a promisingly candidate to alloy with the metallic core because of its depletion in the crust and the mantle relative to other volatile elements by several orders of magnitude (e.g., [3 -5]). In the last decades, several experimental studies have aimed to quantify the sulphur content in the Earth's core and to determine its influence on the physical properties (e.g., [6]). However, experimental data on sulphur partitioning between silicate and metallic liquids at pressures and temperatures relevant for core-mantle boundary conditions are missing. This lack is due to pressure and temperature limitations of conventional experimental approaches (up to 25 GPa and 2200 K). New developments, like laser-heated diamond-anvil cells (LDAC), allow studies at core-mantle boundary conditions, but in-situ chemical analysis of sulphur in LDACs is impossible due to the high absorption of S fluorescence in the diamonds. Instead of sulphur, selenium can be used to model sulphur partitioning between silicate and metallic melts at elevated PT conditions. This is based on the fact that sulphur and selenium can be considered as geochemical twins ([7,8]). The main advantage of this approach is the much higher excitation energy of selenium compared to sulphur, which enables in-situ XRF analysis in LDACs.

Here, we present data on Se partitioning between silicate and metallic melt at extreme conditions. The experiments have been performed in double-sided laser-heated LDACs at the high pressure beamlines P02.2 (DESY, Germany) and ID27 (ESRF, France) as described in [9]. Micro-XRF mappings are used to visualise changes of the Se distribution before and after laser heating. Micro-XRD is used to determine the experimental pressure, the onset of melting and also provides information on distribution of high-pressure / high temperature phases (XRD map). In order to fully apply the observed in-situ Se results to the S partitioning, the recovered samples are additionally analysed ex-situ for Se and S by XRF, EMP, and HRTEM. This will also set constraints on the effect of quenching.

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9.5: **Key characteristics of the Fe-snow regime in planetary cores**

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In view of the fact that Ganymede shows signs of an internally produced magnetic field [1] the search of its origin became a scientific challenge. For small planetary bodies such as Ganymede the iron snow regime, i.e. the top-down solidification of iron, has been suggested to play an important role in the core cooling history [2,3]. In that regime, iron crystals form first at the core-mantle boundary (CMB) due to shallow or negative slopes of the melting temperature [3]. The iron crystals are heavier than the surrounding Fe-FeS fluid, which causes them to settle. In thermo-chemical equilibrium a stable chemical gradient arises within the precipitation zone and the solid iron particles will redissolve in deeper core regions, whenever the core temperature is higher than the melting temperature. Redissolving of the iron particles forms a dense Fe-rich fluid on top of a lighter Fe-FeS fluid. That corresponds to a gravitationally unstable situation. We propose that this could be the starting point for compositional convection within the deeper core regions of Ganymede, which may be the driving mechanism for the potential core dynamo. However, as soon as the precipitation zone is present within the entire core and an inner core starts to grow that kind of compositional convection would stop. According to that dynamo action would be restricted to the time period of growing the precipitation zone across the entire core. In the scope of a 1D thermo-chemical evolution model, we investigate the key characteristics of the iron snow regime within Ganymede's core. Those key characteristics are the compositional density gradient evolving across the precipitation zone and the time period necessary to grow the precipitation zone across the entire core. We find that all tested scenarios would require strong superadiabatic cooling for thermally driven overturning convection. The investigated time periods to grow the precipitation zone across the entire core can differ from 220 to 939 Myr. Since Ganymede seems to have a core dynamo, which is active today, these findings mean, that the iron snow regime should have started late in Ganymede's thermal history. Since higher core sulfur concentrations yield larger time spans, we argue that the sulfur concentration of Ganymede's core should be close to the eutectic. Furthermore, according to the above proposed mechanism the existing dynamo suggests that Ganymede has no present-day inner solid core.

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9.6: **Carbon under Extreme Conditions**

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Carbon and carbon compounds play an important role in the chemistry and physics of planets. In Neptune and Uranus for example the abundance of carbon in the form of methane amounts to 10-15% of the total mass. It was shown that methane can dissociate under the extreme conditions in the interior of these planets and may precipitate in the form of diamond [1]. Another example is the extrasolar super-Earth 55 Cancri e which has recently been discussed to contain 10-70% of carbon [2] leading to a planet that consists perhaps of a huge amount of diamond.

The modeling of the interior structure of such planets requires precise knowledge of the phase diagram and equation of state (EOS) of carbon in a wide range of pressures and temperatures. A variety of high pressure phases have been proposed including the BC8 phase at pressures above 1 TPa followed by a simple cubic (SC) phase above 2.9 TPa [3], which have yet to be experimentally confirmed.

In our work we investigate the diamond-BC8 coexistence line for temperatures up to 7000 K using the Vienna Ab Initio Simulation Package (VASP [4]). The transition pressure is obtained from the free enthalpies of the respective phases. We take into account the vibrational entropies by calculating phonon dispersions with Phonopy [5]. Results are compared with other theoretical calculations.

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9.7: **Ab initio simulations for the structure factor of liquid and warm dense aluminum**

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We perform finite-temperature DFT-MD simulations to determine the static and dynamic structure factor of aluminum. The results are compared to experimental x-ray scattering data on liquid aluminum where very good agreement is obtained. Furthermore, we calculate the dynamic structure factor from the autocorrelation function of the Fourier transformed ion density. We extract the dispersion relation of the collective excitations for both liquid and warm dense aluminum and determine the corresponding speed of sound.

9.8: **Calculation of the 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 different elements like beryllium [2,3] or boron [4,5].

We calculate the structure factor by means of it ab initio molecular dynamics simulations. The static structure factor is obtained via the pair distribution function. While the dynamic conductivity is derived from the Kubo-Greenwood formula [6], and a Drude-like behaviour is observed. The corresponding dielectric function is used to determine the dynamic structure factor. We present results for the static structure factor for boron and the dynamic structure factor for beryllium and compare with perturbative treatments such as the Born-Mermin approximation.

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9.9: **Monte Carlo simulations of ionization potential depression in dense plasmas**

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Particle-particle Monte Carlo (MC) model with coulomb pair potential interaction was used to simulate the modification of ionization potentials by electrostatic microfields. The Barnes-Hut algorithm was used to speed up the calculations of the electric potential. Atomic levels were approximated to be independent of the microfields as was assumed in the original paper [1] by Ecker and Kröll (EK); however, the available levels were limited by the corresponding mean inter-particle distance. The code was tested on dense hydrogen plasmas and a reasonable agreement was found in both the Debye regime, and in the high density limit. In the high density limit it resembled more the modified EK (mEK) model (with C=1) [3,4] than the more often used Stewart and Pyatt (SP) model [2]. The MC model was also used for aluminum plasmas where it gave consistently lower depression values then the mEK model simulations presented in [3,4]. The MC gave slightly better (higher) depression values than the SP model simulations as presented in [4]. As no fitting or adjustments were done, the achieved level of agreement justifies us to say that the statistical physics model of EK is theoretically sound.

Most probably the step of the calculation connecting the chemical potential and the greatly simplified spatial charge distribution around an ion in the original EK paper suffers from some problems, giving their constant C which was not good enough. This motivated later authors to modify it.

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9.10: **Thermal evolution of Saturn considering H-He-demixing**

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Saturn is a very interesting object in our solar system. Especially the cooling history of this planet and its luminosity propose conundrums. Measurements from the Voyager mission show that Saturn radiates about twice the energy back into space than it receives from the sun [1]. Calculations describing the cooling behavior based on a homogeneous evolution of Saturn have already been done and yield ages of 2 – 3 billion years for the age of this planet [2,3]. Compared to the age of the solar system of about 4.56 billion years this is much too short what means that the planet cools out too fast. We present a thermodynamically self-consistent model including the demixing of hydrogen and helium. When the isentrope enters the demixing region, helium rain may occur and additionally heats the planet via the release of gravitational energy [2,4]. As a result our models predict a nearly pure helium layer directly above the planetary core. We describe the growth of this shell in mass and thickness with respect to the inhomogeneous evolution of Saturn.

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9.11: **Determinability of the Love-number k_2 of Exoplanets from Transit Timing Variations**

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The big majority of exoplanets were discovered either via radial velocity measurements, which give only a lower mass-limit for the exoplanets, or via transit photometry, which gives the inclination and the radius of the planet. A combination of these two methods allows us to measure the mass, radius and mean density of exoplanets for transiting exoplanets. However, these two independent parameters (mass and radius) do not constrain fully the exoplanetary interior.

Measuring Transit Timing Variations (TTV) may provide an additional constrain into the interior-studies, because some of the orbital parameters vary due to the tidal-interaction between the star and the planet, and this causes a variation in the orbital period of the planet which is measurable via the TTV-method. The basics of the method and its applicability and the futue prospects are reviewed in this talk. Contributions of ground-based and space-based (CoRoT, Kepler and PLATO) observations are also summarized.

9.12: **Investigation of plasma jet creation and collimation mechanisms**

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In astrophysics, supersonic collimated outflows from gravitating sources are a common occurrence. The jet structure has been the subject of several simulations, observations and theories and is thought to be best described as a multicomponent structure, composed of a dense central region surrounded by a thin cocoon, therefore being highly complex.

In this context, the possibility to simulate the jet formation using high power lasers bears large potential. A number of previous experiments have proven successful in developing optimized target geometries for creating jets and investigating various stages of their evolution.

Here we present recent studies dedicated to the investigation of collimating effects. We will consider different processes presumed to play a role in the collimation mechanism. In particular we will discuss the influence of inhomogeneous environments, such as surrounding outflows of different density and composition and quasi-stationary gas flows. Using an ensemble of optical and X-ray diagnostics we can access both the thin outer part of the jet and the denser core, thus achieving an extensive measurement of the jet characteristics.

In addition, recent developments on experimentally investigating the influence of external magnetic fields using pulsed coils are discussed.

9.13: **Current status and future plans for the Extreme Conditions Beamline (ECB), P02.2, PETRA III, DESY**

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2012 was the first year of general user operation for the Extreme Conditions Beamline (ECB) P02.2 at PETRA III and accepted a total of 54 users. During this time, we have also commissioned the "General Purpose" setup dedicated to experiments in the resistively heated and cryogenically cooled DAC. Finally, we extended the energy range that we are able to offer to users by adding fixed energies of 60.0 and 77.1 keV. Within this poster, we present some of the current characteristics/capabilities and give an outlook on what we are planning for 2013 and the PETRA III extension shutdown to enhance the capabilities of the ECB.

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We look forward to meeting you at the

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- evolution and structure of giant planet interiors,
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