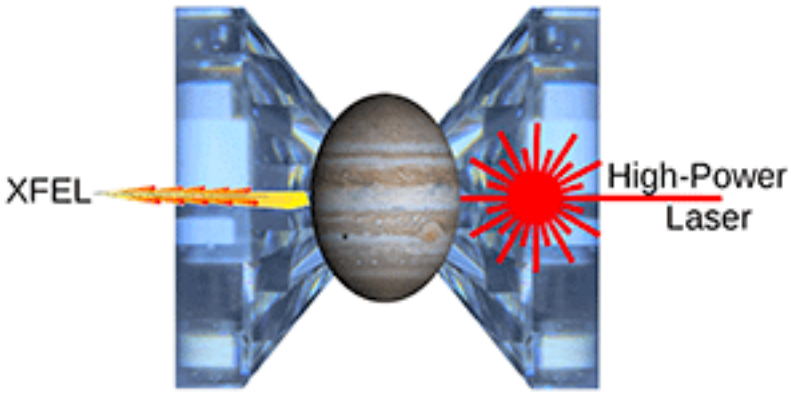
8th Joint Workshop on High Pressure, Planetary and Plasma Physics (HP4)

Wednesday 09 October 2019 – Friday 11 October 2010

Dresden



Book of Abstracts
(Draft: 03.10.2019)

Oral presentations

Water World Galore

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Exoplanet radii show a bimodal distribution, with two peaks corresponding to smaller planets (likely rocky) and larger intermediate-size planets, respectively. We apply interior structure model, growth model, as well as atmospheric escape model, and conduct Monte Carlo simulations, to demonstrate that many intermediate-size planets are water worlds. This result has profound implications on planet formation theory and origins of life. (https://arxiv.org/abs/1906.04253)

Viscosity and Prandtl Number of Warm Dense Water as in Ice Giant Planets

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The thermophysical properties of matter in water-rich planets are important for understanding their radius, luminosity, and magnetic field. Here we present theoretical predictions for the thermal conductivity, viscosity, and Prandtl number (P_r) of warm dense water at conditions present in mini-Neptune to Neptune-sized planets (0.2 - 6 g/cm^3, 1000 - 50000 K). These transport properties were derived from ab initio molecular dynamics (MD) simulations based on density functional theory (DFT) by evaluating Kubo-Greenwood and Green-Kubo expressions in various post-processing calculations [1,2,3]. As a general result, we find that P_r is equal to or greater than 1 in their deep interiors if they are adiabatic, whereas P_r is smaller than 1 if they are super-adiabatic. Our findings lend some support to the suggestion of turbulent convection at $P_r \sim 1$ to explain the peculiar magnetic fields of Uranus and Neptune. Finally, we argue that double-diffusive convection in these Ice Giants would require fine-tuning of the compositional-to-superadiabaticity ratio R_{crit} within a small factor of 2; instead we conclude that compositional gradients in Uranus and Neptune would be diffusive in nature and, thus, primordial heat could still be trapped inside. Our results are important for the development of non-adiabatic convection and evolution models for water-rich giant planets like Uranus and Neptune.

This work is supported by the DFG within the FOR 2440 “Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics.”

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Thermal evolution of Uranus and Neptune

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Uranus and Neptune have highly different intrinsic heat fluxes. This is surprising since they share a large number of very similar observed values such as mean density, surface temperature and atmospheric composition. Moreover, previous evolution calculations fail to reproduce the present-day luminosity of Uranus, or - equivalently - yield too long cooling times [1,2]. Here we investigate how different equations of state for H/He and for water affect the luminosity of assumed adiabatic models. We find that application of H/He-REOS.3 [3] yields about 0.7 Gyr (Neptune) and about 1.8 Gyr (Uranus) shorter cooling times for the ice giants compared to the previously used H/H-REOS.1 [4] and Sesame 7150 EOS [5]. This trend is confirmed if we apply the recent EOS by Mazevet et al for water [6]. As a result, adiabatic Neptune appears too bright for its known age.

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H2O Ice at High-Pressure and -Temperature studied by X-Ray Diffraction in a Resistively Heated dynamic Diamond Anvil Cell (RHdDAC)

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Dynamic compression experiments across the phase transition between ice VII and ice X were performed at room and high temperatures at the Extreme Conditions Beamline (ECB) at PETRA III. A dynamic Diamond Anvil Cell (dDAC) driven by a piezo electric actuator [Evans et al. 2007; Jenei et al. 2019] has been equipped with a resistive heating system to perform compression at high temperatures. The combination of the RHdDAC with extremely sensitive GaAs LAMBDA detectors available at the ECB facilitates time-resolved x-ray diffraction measurements along the compression ramps. Compression rates were set to approx. 0.3 GPa/s in order to be able to employ relatively long exposure times (0.5 and 1 second) on the LAMBDA detectors, ensuring a good signal to noise ratio of the integrated diffraction patterns. DAC were assembled with 150 mm culet anvils and an amorphous gasket out of metallic glass. The gasket material was drilled with a 50 µm diameter hole where liquid H2O was loaded together with a pressure marker (i.e. gold powder). We ran 4 compression ramps at 600, 800, 1000 and 1200 K reaching pressures up to 90 GPa. Experimental times were limited to approx. 40 minutes, including heating and compression, in order to prevent heat transfer to the piezo electric actuator and reaction between sample and gasket. Crystallization of the amorphous gasket or products of reaction between H2O and the gasket material at high temperatures were not observed in any of the experiments. Additionally, we ran 3 compression ramps at room temperature achieving pressures of about 200 GPa. Pressure-volume data were derived from the diffraction peaks of Au (111) and Ice (110). According to previous experiments employing different characterization techniques, the ice VII - dynamic ice VII – dynamic ice X transition takes place at pressures from 30-60 GPa [Wolanin et al. 1997; Song et al. 1999; Grande et al. 2019]. Recent Brillouin scattering measurements have reported a softening of the elastic bulk modulus (K) of ice in the same pressure range [Li et al. 2019]. We observed in our data a continuous change in the slope of the P-V curve of H2O ice starting at a pressure of about 35 GPa at ambient condition that is indicative for a phase transition. According to the expression of the isothermal bulk modulus K=-V (dP/dV), we can observe the elastic response of ice across the phase transition by differentiating the P-V data. A softening followed by a hardening of the bulk modulus is observed over the pressure range from 35-60 GPa at room temperature. Analysis of the effect of temperature on the mentioned phase transition is under way. The direct measurements of the bulk modulus are crucial for future modelling of the geology of Ice Giants, Uranus and Neptune as well as mini-Neptune exoplanets.

Laser-driven compression of water, ammonia, and C:H:N:O mixtures of interest for Icy Giants interiors

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The icy giants Uranus and Neptune remain the least characterised planets of our solar system. Building reliable models of their interior structures is crucial to address their formation and evolution, as well as to interpret astronomical observations of magnetic fields, luminosity and gravitational moments. As today, our modelling capabilities of icy giants is heavily hindered by the poor characterisation of their principal component, the so called "planetary ice", at the extreme pressure and temperature conditions of their interiors. Far from being the frozen solid we are familiar with, the "planetary ice" is rather a mixture of water, ammonia and methane. The physical and chemical properties of such mixtures at multi Mbar and few thousands K is not only important for planetology but they are also interesting on their own, since those conditions are characterized by the coexistence of dissociated atoms, atomic clusters and polymer chains. This regime is very difficult to study via ab initio simulations and experimental verifications are thus required.

Here we present the results we obtained using laser-based compression schemes on water, pure liquid ammonia, and a C:H:N:O mixture composed by water, ethanol, and ammonia. Their principal Hugoniot curves have been explored using decaying shocks, while off-Hugoniot states have been reached via a double-shock technique and through the coupling of dynamic and static compression in diamond anvil cells. The experiments were performed at the LULI2000 laser facility using standard rear-side optical diagnostics (VISARs, SOP). The equation of state and the optical reflectivity of the shock front have been measured and compared to ab-initio calculations.

Polystyrene at Extreme Pressures

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Using the SG-III prototype laser at CAEP, Mianyang, we have measured the conditions of polystyrene samples driven to conditions on the principal Hugoniot up to P˜1 TPa (10 Mbar), and away from the Hugoniot up to P˜300 GPa (3 Mbar). The response of the samples was measured with a velocity interferometry diagnostic to determine the material and shock velocity, and hence the conditions reached, and the reflectivity of the sample, from which changes in the conductivity can be inferred. By applying the self-impedance mismatch technique with the measured velocities, the pressure and density of thermodynamic points away from the principal Hugoniot were determined. The results demonstrate an anomalously high reflectivity at extreme shock pressures, with the off-Hugoniot states showing a low conductivity due to the reduced temperature.

Development of a high-quality X-ray Scattering and X-ray Raman Spectroscopy setup for the characterization of warm dense carbon at the HED instrument of EuXFEL

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Warm dense matter (WDM) states are high-pressure high temperature states characterized by a thermal energy that is comparable to the bonding energy of matter. This causes partial ionization, electron degeneracy and ion coupling, which makes model calculations very challenging. The precise characterization of the microscopic properties of WDM is not only extreme ambitious theoretically but also experimentally. Bright X-ray sources, like X-ray free electron laser (XFEL), in combination with high-power high-energy optical laser provide unique possibilities for creating and probing these extreme material states in the laboratory. However, the applied diagnostics require usually theoretical models as an input for the data analysis. Thus, simultaneous measurements with complementary diagnostics, like spectrally resolved X-ray scattering (XRTS), X-ray diffraction (XRD), X-ray absorption spectroscopy (XAS) and more, are highly desirable for obtaining a complete understanding of warm dense matter and their structural and electronic properties. As most abundant inside giant planets, the investigation of low-Z elements under WDM conditions plays a crucial role in planetary physics. Additionally, they are theoretically accessible reasonably well, due to their low number of electrons. However, applying X-ray absorption spectroscopy techniques to an experimental setup investigating dynamically compressed low-Z element samples involves difficulties due to the low energies of the K-edges that require the use of soft X-rays and therefore thin targets. X-ray Raman Spectroscopy instead is an alternative technique, which provides equivalent information and can be performed with hard X-rays and therefore bulk targets that are required for shock compression experiments. The small cross-section of the scattering process can be overcome by using data accumulation in high-repetition-rate experiments. Beginning 2019, the High Energy Density (HED) instrument at the European X-ray Free Electron Laser (EuXFEL) has started to be established. While first experiments have been performed using an X-ray-only configuration, the installation of high-power optical drive laser is in progress, which will present outstanding opportunities for an extensive investigation of warm dense matter. This talk presents very recent results from one of the first experiments at the new facility, where we demonstrate an experimental setup, which combines high-quality X-ray scattering techniques together with X-ray Raman Spectroscopy studying samples composed of carbon and shows the unique capabilities and future possibilities of HED.

Ab-initio dielectric response function of diamond and high-pressure phases of carbon

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The description of the electronic and ionic properties of carbon, of the equation of state (EOS), and the corresponding phase boundaries requires state of the art ab-initio methods such as density functional theory (DFT) with molecular dynamics (MD) or path integral Monte Carlo. A combination of DFT and many-body quantum statistics allows to include higher order correlations and describe new physics such that the accuracy and predictive power of theoretical methods is enhanced. We are particularly interested in the dynamic structure factor (DSF) as it is an important quantity to determine properties of high-pressure solids and fluids and warm dense matter states. The DSF can be accessed, e.g., using energetic x-ray free-electron (XFEL) radiation or electron beams. Enhanced DSF models include in particular electron-hole interactions in semiconductors and insulators. This provides improved predictions for dielectric functions and conductivities, especially when it is combined with higher rungs of xc-functionals for a better description of the band gaps. From these, better EOS may be derived based on the DSF or dielectric function. As a practical application, the determination of the temperature based on X-ray Thomson scattering (XRTS) data will be improved. The dielectric response function of the diamond, body centered cubic diamond (bc8), and hexagonal diamond (lonsdaleite) phases of carbon are computed using density functional theory and many-body perturbation theory with the emphasis on the excitonic picture of the solid phases relevant in the regimes of high-pressure physics and warm dense matter. We also discuss the capabilities of reproducing the inelastic x-ray scattering spectra in comparison with the existing models in light of recent x-ray scattering experiments on carbon and carbon bearing materials in the Megabar range.

The Deep Winds of Jupiter and Saturn As Inferred from Recent Gravity Measurements: Similarities and Differences

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The two gas giants of the Solar System, Jupiter and Saturn, exhibit strong zonal flows at the cloud level. The Jupiter winds consist of strong zonal jets (up to 140m/s) alternating latitudinally between eastward and westward jets, and have a significant asymmetric component between the northern and southern hemispheres. On Saturn, the wind pattern is a wide and mostly symmetric eastward flow of nearly 500 m/s at the equatorial region, and smaller scale jets extend to high latitudes. But how deep these winds penetrate into the planets interior remained a fundamental open question until recently, when both Juno at Jupiter and Cassini at Saturn enabled answering this decades long question. The gravity experiments, performed by both spacecrafts, provided measurements of the gravity harmonics with unprecedented accuracy. They brought into light substantial differences between the two planets. Using the gravity measurements, together with an adjoint based inverse model of the large-scale flow dynamics, we find that on both planets the winds are very deep - reaching around 3,000km on Jupiter and around 9,000km on Saturn. This points to some similarities and differences between both planets. On both planets, the winds observed at the cloud level are a manifestation of deep flows extending thousands of kilometers deep. With that, the differences are striking. The winds on Saturn, a planet smaller than Jupiter, penetrate 3 times deeper and are much more symmetric than the winds on Jupiter. The winds on Jupiter, penetrating to lesser depths, seems to be less connected between the hemispheres, and thus allowing stronger asymmetries to evolve. These differences are likely the result of Saturn having a 3 times smaller mass and a much weaker magnetic field. In the presentation we will discuss the depth of the winds analysis, and the implications to the characteristics of the two planets.

Light elements under extreme pressure

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Hydrogen and helium together constitute about 98% of all the visible matter in the Universe, and are the major components of astrophysical bodies. In these bodies, hydrogen and helium are subject to extreme conditions of pressure and temperature, which leads to physical and chemical properties that differ significantly from the corresponding ambient conditions properties.

In this talk, I will describe our quantum mechanical calculations to understand the phase diagrams of hydrogen and helium under giga and terapascal pressures. We find that hydrogen has a rich and complex solid phase diagram, and will pose the question of how metallisation occurs in this element. We also find that helium can form compounds with other elements at sufficiently high pressures, forcing us to revisit our understanding of this textbook inert gas.

Linking Zonal Winds and Gravity: The Relative Importance of Dynamic Self-Gravity and non-polytropic Interior Models

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Recent precise measurements of Jupiter's and Saturn's gravity fields constrain the properties of the zonal flows in their outer envelopes. A simplified dynamic equation establishes the link between zonal flows and the related buoyancy perturbation, where the latter comprises of a dynamic density perturbation and a dynamic gravity perturbation. Whether or not the action of the dynamic gravity perturbation needs to be explicitly included in this equation, an effect we call the Dynamic Self Gravity (DSG), has been a matter of intense debate. We show that for polytropic interiors the full equation can be solved (semi) analytically in terms of the gravity potential. This allows us to quantify the impact of the DSG on each gravity harmonic, practically independent of the zonal flow. The impact decreases with growing spherical harmonic degree l: for degrees l=2 to about l=4, the DSG is a first order effect, whereas for degrees of about l=5 to roughly l=10, the relative impact of DSG is about 10% and hence significant.

If more realistic ab-initio interior models are considered the DSG is multiplied with a radius dependent function, requiring to solve a 2nd order ODE. We introduce two numerical frameworks, both yielding rapid and accurate solutions to the full problem. Further, we calculate the leading order gravity moments induced by Jupiter's antisymmetric zonal flows and quantify the effect of utilizing a realistic ab-initio interior model in favor of a simple polytrope of index unity. Our results indicate that both, the interior model and the DSG, potentially introduce an offset of up to 30%. However, in opposite to the DSG, the relative importance of the interior model does not seem to vanish at higher degrees. Hence, both effects should be taken into account in any attempt of inverting gravity measurements for zonal flow properties.

Planetary dynamos in the lab

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Magnetic fields of planets are known to be generated by the homogeneous dynamo effect in moving liquid metals, such as iron or metallic hydrogen. For a long time, hydromagnetic dynamos have been the subject of purely theoretical and numerical research. This situation changed in 1999 when the threshold of magnetic-field self-excitation was crossed in the two large-scale liquid sodium experiments in Riga and Karlsruhe. Since 2006, the VKS dynamo experiment in Cadarache has successfully reproduced key processes of geophysical interest such as reversals and excursions. Further liquid metal experiments in Grenoble, Madison, Maryland, Perm, Princeton, Perm, Queretaro, and Socorro have contributed important findings to dynamo research. After giving an overview about those recent achievements, the talk will delineate the present status of the DRESDYN precession experiment at HZDR. A few further issues connected with theexperimental demonstration of magnetically triggered flow instabilities, such as magnetorotational and Tayler instability, are also discussed.

Mass Transport and Structural Properties of Binary Liquid Iron Alloys at High Pressure

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We determine mass transport and structural properties of binary liquid iron alloys over a wide density (5.055–11.735 $g \cdot cm^{-3}$) and temperature range (2,500–6,500 K) using first-principles molecular dynamics. Compositions consist of 96 at% Fe and 4 at% φ, where φ = H, C, N, O, Mg, Si, S, or Ni. Self-diffusion coefficients (D) of Fe and φ range from $3.5 \cdot 10^{-9}$ to $1.9 \cdot 10^{-7}$ $m^2 \cdot s^{-1}$. Results show a relation between mean atomic radius and diffusivity ratio for the alloying element and iron: Si and Ni are "iron-like" with similar atomic radii and D compared with those of Fe; H, C, N, O, and S are "small non-iron-like" with smaller atomic radii and larger D; and Mg transitions from "large non-iron-like" with a larger atomic radius and smaller D at low density to iron[U+2010]like under conditions of the Earth's core. The effect of pressure on D for C, N, and O is negligible for densities below ~8 $g \cdot cm^{-3}$, accompanied by an increase in average coordination numbers to ~6, and an increase in mean atomic radii. For densities above ~8 $g \cdot cm^{-3}$, diffusivities and atomic radii of these elements decrease monotonically with pressure, which is typical for the iron-like alloying elements as well as for H, Mg, and S over the whole compression range. While atomic radius ratios move toward unity with compression, diffusivity ratios for the alloying element relative to iron tend to increase for the "non-iron-like" elements with density.

Explaining Jupiter's Peculiar Magnetic Field

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The magnetometer on NASA's Juno spacecraft has revealed peculiar details of Jupiter's magnetic field. While the field is dominated by the axial dipole component, it also shows pronounced field concentrations in a latitudinal band in the northern and a single 'blue spot' in the southern hemisphere unlike any other planetary field in our solar system. What do these features tell us about the dynamo operating in Jupiter's interior? Here we show that such features are produced where the zonal winds observed at cloud level reach down to sizable electrical conductivities in numerical dynamo simulations of Jupiter's dynamics. The connection is established with data assimilation techniques that exploit the statistical correlations in the dynamo simulation. These correlations allow us to predict the dynamics deeper in the planet. At least the equatorial zonal jet must reach down to about 95% of Jupiter's radius but with at much reduced amplitude in the order of centimeter per second. The jet gives rise to a secondary dynamo that significantly modifies the large-scale field produced deeper in the planet. Spotting features are Jupiter-like banded structures that travel from low to high latitude in the form of Parker dynamo waves and local instabilities similar to the 'blue spot'. Our work is the first application of data assimilation techniques to the dynamo of other planet's than Earth. The lack of comparable magnetic features in other planetary magnetic fields suggest that the winds are either too weak (Earth) and/or do not reach deep enough (Saturn, Uranus, Neptune).

Present status and future prospects of exoplanetary Love number measurements from radial velocities and from transit timing variations

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Exoplanets Love number

Investigating exoplanet interiors from transit light curves

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The Love numbers h_2 and k_2 provide invaluable additional constraints on planetary interiors, when combined with mass and radius (Kellermann et al., 2018; Padovan et al., 2018). They help breaking the degeneracy between mean density and density profile: for instance the Earth and Mercury exhibit similar mean densities but different Love numbers, illustrating their opposite internal composition (Lambeck, 1980; Konopliv et al., 2019). Such measurements would be of great importance for exoplanetary studies, e.g. in discriminating super Earths from mini Neptunes. Planets orbiting close to their host star will undergo strong tidal and rotational deformations, function of h_2, which modify their shape from spherical to more complicated ones (Love, 1911). We first summarize the planetary shape model. Taking the hot Jupiter WASP-121b as a case study, we then present how h_2 can be measured from transit observations in the light of dedicated past, current and future facilities (Hellard et al., 2019). In particular, we show that the photometric precision should be higher than 90 ppm/min and the uncertainty on the stellar limb darkening coefficients smaller than 0.01 to confidently retrieve h_2 from transit light curves. We translate those requirements into a required number of observed transits to emphasize the capability of several telescopes to measure h_2. The knowledge of Love numbers for exoplanets, combined with their mass and radius, will greatly increase our understanding of their formation, evolution, and interiors.

Ways to improve our understanding of exoplanets' interiors

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What we know of the interior structure and history of the handful of planets of the solar system is based on an extensive amount of remote sensing data, in-situ observations, and direct samples. In the field of exoplanets, the situation is complementary, where only a handful of constraints are available for a given planet, but already more than 4000 objects have been identified. Thus, to further our understanding of the interior structure and evolution of exoplanets, two approaches could be pursued: trying to increase the number of constraints and trying to take advantage of the large number of objects observed. One new constraint that will be available for an increasingly large number of exoplanets is the Love number k_2, which is proportional to the radial mass concentration of the planet, a key information to investigate the interior structure. The analysis of the large amount of data for exoplanets can be approached in a big-data framework, which provides a clear way to assess the information content of exoplanet observational constraints. Recent results based on the combination of the Love number constraint with a big-data analysis tool will be presented.

The Effect of Clouds as an Additional Opacity Source on the Inferred Metallicity of Giant Exoplanets

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Atmospheres regulate the planetary heat loss and therefore influence planetary thermal evolution. Uncertainty in a giant planet's thermal state contributes to the uncertainty in the inferred abundance of heavy elements it contains. Within an analytic atmosphere model, we here investigate the influence that different cloud opacities and cloud depths can have on the inferred metallicity of irradiated extrasolar gas giants. For that purpose, we perform coupled atmosphere, interior, and evolution calculations. We show that optically thick, high clouds have negligible influence whereas deep-seated, optically very thick clouds can lead to warmer deep tropospheres and therefore higher bulk heavy element mass estimates. For the young hot Jupiter WASP-10b we find a possible enhancement in inferred metallicity of up to 10% due to possible silicate clouds at ~0.3 bar. For WASP-39b, whose observationally derived metallicity is higher than predicted by cloudless models, we find an enhancement by at most 50%, confirming the conclusion of a further energy source at work in this planet.

Behaviors of carbon in extreme conditions

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Carbon is one of the great interests of researchers in the broad area of material sciences, being used also in a lot of HED experiments. We here present the recent experimental results on particularly carbon and carbon mixture materials in extreme conditions; 1) observations of the compression process and deformation anisotropy in full dense, highly transparent nano-crystalline diamond; 2) possibility of chemical reactions in carbon mixture materials. The status of the HEDS platform at SACLA is also reported.

The XFEL experiments were performed at the BL3 of SACLA with the approval of Synchrotron Radiation Research Institute (proposal Nos. 2017A8062, 2017B8051, 2018A8036, and 2018B8069). This work was supported in part by Japan Society for the Promotion of Science (JSPS) KAKENHI (grant nos. 16H02246 and 19K21866) and the Q-LEAP Flagship Program (JPMXS0118067246) at Osaka University from the Ministry of Education, Culture, Sports, Science, and Technology (MEXT).

The High-Energy Density instrument at European XFEL: Current status and X-ray performance

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The High-Energy Density instrument at European XFEL (HED) is an instrument dedicated to study short lived extreme states of matter with hard X-ray FEL radiation [1,2]. HED is located at the SASE2 hard X-ray undulator that is designed to provide photon energies in the range of 3 to 25 keV and allows probing with fs short X-ray pulses with repetition rates of up to 4.5 MHz. After a long construction period, SASE2 delivered first X-ray radiation in May 2018. Subsequently, major parts of the X-ray beamline were commissioned and first FEL radiation entered the optics hutch right ahead of the FEL shut down at beginning of December. In early 2019, the optics hutch and interaction area 1 were completed for first user experiments. Commissioning of the X-ray components resumed after the FEL restart in mid-February to prepare the first three user experiments that took place from May 15th - June 6th. Currently, the instrument is in the second user run that will last until mid-November 2019. While the first set of experiments were either advanced commissioning experiments of the X-ray performance or use the FEL beam directly as a driver, work on the optical drive lasers is being performed in parallel: the Amplitude 10 Hz short pulse laser system was delivered to HED in May 2018 and is currently in its commissioning phase. The 10 Hz long pulse Dipole laser D100X is currently being tested at The Centre for Advanced Laser Technology and Applications (CALTA) at the Central Laser Facility, UK and recently demonstrated lasing at 100 J. The delivery to European XFEL is expected for 2019. The generic pump-probe laser developed by the European XFEL laser group [3] demonstrated the ability to work at up to 4.5 MHz. The respective laser system for HED will be installed from 2019. In addition to information on latest beamline performance and optical laser status, this contribution will highlight some commissioning results of the first run time, like energy dispersion of the instrument and photon beam characteristics. Finally, the two main experimental chambers (IC1 and IC2) and the status of X-ray techniques are presented.

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Femtosecond laser produced periodic plasma in a colloidal crystal probed by XFEL radiation

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With the rapid development of short-time intense laser sources, studies of highly excited matter under extreme irradiation enter further unexplored regimes. In addition, an application of freeelectron laser, delivering intense femtosecond pulses of X-ray radiation as a probe in contemporary IR pump - X-ray probe experiments enables to investigate non-equilibrium stages of sample evolution with an unprecedented time resolution. In this work we present the detailed study of the IR-pumped and X-ray probed periodic plasma created from the colloidal crystal. Both experimental data and theory modeling show that the periodicity present in the sample survives to a large extent the extreme excitation and shock wave propagation inside the colloidal crystal on hundreds picosecond timescale. This feature enables probing the excited crystal even at those very long timescales, using the powerful Bragg peak analysis. This is in contrast to the conventional studies of dense plasmas created after amorphization of bulk samples for which such long-timescale probing with Bragg diffraction technique is not possible. X-ray diffraction measurements of excited colloidal crystals may then open a new pathway for studies of warm dense matter and plasma, leading towards a better understanding of matter transitions under extreme irradiation.

Present and future of X-ray scattering techniques for the understanding of ultra-short pulse laser matter interactions

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The development of next generation laser plasma sources for novel applications in various fields ranging from astro-physics, fusion research to particle acceleration and tumor therapy requires methods to study the plasma dynamics and heating on short spatial (few nanometers) and temporal scales (few femtoseconds). Free electron lasers are identified as a potential new tool to achieve this goal for various plasma properties since they combine short bunches, high photon numbers with small bandwidth and high penetration power even through several microns of solid density plasmas. We give an overview over recent advances in theory and experiments for transferring established scattering techniques into the short-pulse laser domain. Besides the future potentials of the small angle scattering technique we will focus on the possible impact of resonant scattering on the understanding and advancement of laser-based particle sources. The simultaneous measurement of structure and opacity with a single method, with nanometer and femtosecond resolution would enable a level of understanding both in plasma physics as well as transient, non-equilibrium atomic physics that could help developing better redictive simulation capabilities as well as new solutions to defiances towards optimized laser particle sources.

Structure, equation of state, and phase transitions in shock-compressed minerals to TPa pressures

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Dynamic compression studies of minerals have applications to understanding planetary formation, shock metamorphism, and high-pressure phases of deep planetary interiors. Historically, measurements under in situ shock-loading conditions have been restricted to acquiring only continuum-level information and the lattice structure could not be determined. Furthermore, features observed in samples recovered from shock experiments can be ambiguous as they may be affected by unloading processes. With the recent development of user facilities combining laser and gas-gun techniques for dynamic compression with x-ray diffraction capabilities, it is now possible to directly probe the atomic structure and observe phase transitions in real time under shock loading. This talk will summarize our recent studies at the Omega Laser (U. Rochester) and the Linac Coherent Light Source (LCLS). At Omega, the laser drive can be used to compress minerals up to TPa pressures allowing us to probe the nature and kinetics of structural phase transitions on nanosecond timescales. At LCLS, laser-compression combined with free-electron x-rays is used to explore the behavior of minerals up to 150 GPa. By carrying out a series of pump and probe experiments the structural evolution of these materials during shock compressionand release at nanosecond timescales can be constrained.

B1-B2 Phase Transition in MgO from anharmonic ab-initio lattice dynamics at conditions of super-Earth interiors

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The explosive growth in astronomical observations has revealed an unexpected variety of planetary bodies in the universe in terms of radius (R), mass (M) and orbital parameters. In order to characterize these exosolar planets, especially regarding the M-R relations, it is necessary to investigate phase stability fields of material candidates under conditions exceeding the temperature (T) and pressure (P) range of Earth's interior significantly. Especially the non-unique M-R ratios in the overlapping regimes of massive rocky planets (super-Earths) and small ice-giants (mini-Neptuns) complicate the classification in terms of interior structure and composition. The available high-T, high-P data and respective predictions of phase stability fields remain limited, as required P, T conditions are challenging not only in experiments, but also in simulations. In particular, the transition P and Clapeyron slopes of the $MgSiO_3$−ppv breakdown sequence in the MgO-SiO_2 system - proposed to dominate super-Earth mantles−are still not available to the precision necessary for the modeling of planetary interiors. In order to obtain temperature dependent transition pressures from density functional theory (DFT) based simulations, a thermal - or vibrational - contribution to energy (Avib) must be added to the electronic ground-state energy. To date, the standard approach of including vibrational contributions to energy is to make use of the (quasi-) harmonic approximation, where phononphonon interactions are not taken into account and thermal conductivity and expansion are not sufficiently described within the approximation. To overcome these problems, MD as well as LD based approaches have been under development that incorporate anharmonic effects, providing access to the investigation of phase stability fields and thermodynamic properties under extreme P and T conditions. We use the LD-based approaches SSCHA (stochastic self-consistent harmonic approximation) and DAMA (decoupled anharmonic mode approximation) to include this type of corrections in our simulations regarding the B1-B2 phase-transition in MgO. Preliminary results show that the anharmonic contribution to Avib leads to a shallower Clapeyron slope than previously predicted, but are in general agreement with recent predictions.

Ionization Potential Depression in warm dense Be and C/CH plasmas

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The electronic structure of warm dense matter states is governed by screening effects induced by pressure ionization. Hence, the ionization potentia differs significantly from the isolated atom case at those conditions. The standard description of this ionization potential depression (IPD) has been provided by the Ecker-Kröll [1] and Stewart-Pyatt [2] models. However, both theories have been challenged by experiments recently, which has led to a strong debate on how to improve IPD models [3-5].

Here, we present a density functional theory molecular dynamics (DFT-MD) approach to tackle this problem. We calculate the effective ionization degree of warm dense beryllium, carbon, and hydrocarbon plasmas based on the sum rule for the dynamic electrical conductivity [6-7]. Subsequently, we derive a measure of IPD for the different materials for temperatures up to 200 eV and pressures in the Gbar range. Our results can directly be applied for modeling the plasma properties typically predicted in ICF as well as in astrophysical objects such as brown dwarfs and low-mass stars.

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Ab Initio Path Integral Monte Carlo Results for the Dynamic and Static Density Response of Correlated Electrons: From the Electron Liquid to Warm Dense Matter

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Over the last decades, there has emerged a growing interest in warm dense matter (WDM), an exotic state with extreme densities and temperatures. These conditions are relevant for the description of astrophysical objects, laser-excited solids, and the pathway to inertial confinement fusion. Despite the remarkable experimental progress at large research facilities around the globe, a thorough theoretical description of WDM is notoriously difficult due to the complicated interplay of (1) Coulomb coupling, (2) thermal excitations, and (3) quantum degeneracy effects.

In this work, we focus on the uniform electron gas (UEG), one of the most fundamental model systems in physics and quantum chemistry. Although most ground state properties of the UEG have been known for decades, a full thermodynamic description at WDM conditions has only been achieved recently [1] on the basis of ab initio quantum Monte Carlo simulations [2]. In this contribution, we extend these considerations to the dynamic structure factor---the key quantity in X-ray Thomson scattering (XRTS) experiments, which have merged as a standard tool of diagnostics in WDM experiments. More specifically, we have carried out extensive path integral Monte Carlo simulations of the UEG going from WDM conditions to the strongly correlated electron liquid regime to compute an imaginary-time density—density correlation function. The latter is subsequently used as input for a new reconstruction procedure, which allows to obtain ab initio results for the dynamic structure factor including all exchange-correlation effects [3,4]. This has allowed us to compute the first accurate data for the dynamic structure factor for different densities and temperatures, and to gauge the accuracy of previous approximations. Interestingly, at strong coupling we find nontrivial shapes around intermediate wave vectors, which manifest in a negative dispersion relation. Moreover, we present extensive new results and a subsequent machine-learning representation of the static local field correction [5], which is of high importance as input for, e.g., quantum hydrodynamics, electrical and thermal conductivities, advanced XC-functionals for DFT, and the interpretation of experiments.

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Nanosecond freezing of gallium under extreme undercooling rate

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Experiments recently performed using the pulsed-power machine Thor, shocklessly compressing thin liquid gallium (Ga) samples at a range of loading strain rates (10ˆ6 – 10ˆ7 sˆ{-1} and peak pressures (20 – 45 GPa), demonstrate freezing at very high driving force with nanosecond solidification kinetics. Building on a previously developed model for the compression-induced solidification of water to the high-pressure ice VII phase, a transient nucleation and growth theory for the time-dependent phase transition from the liquid to the body-centered tetragonal structure of Ga has been developed and applied toward the analysis of the Ga ramp compression data. Having coupled the solidification kinetics model to the hydrodynamic field equations, numerical simulations reveal an intimate relationship between ramp compression loading rate, wave propagation distance and the observed timescale for solidification kinetics. Simulations of multiple Ga ramp experiments demonstrate nearly quantitative agreement with a single physics-based model, with the high level of accuracy attributed to the explicit inclusion of the liquid-solid interfacial thermodynamics in the kinetics model.

Influence of Spin-Orbit Effects in Optical and XANES Spectra of Transition Metals under Extreme Conditions

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Warm dense matter is an extreme state of matter between solids and plasmas, which can be created in inertia confinement fusion experiments and which is expected to be found in the core of giant planets. To further the understanding of matter under extreme conditions, optical and XANES (X-ray Absorption Near Edge Structure) spectroscopy are commonly used to analyse matter experimentally in a pump-probe scheme. In order to interpret these experimental results and, in turn, to predict electronic transport properties which can not be easily accessed experimentally, theoretical description are necessary. In the present work, we simulate transition metals under extreme conditions using quantum molecular dynamics calculations provided by the ABINIT package. To further improve accuracy, we modified the ABINIT DFT code to include the effects of spin-orbit coupling in the calculation of optical and XANES spectra. We will present Cu XANES and Au optical spectra at different electron and ion temperatures, respectively.

Poster presentations

DFT+U equation of state for iron oxide

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The number of detected exoplanets and the capabilities of identifying small, Earth-sized planets have grown tremendously over the last two decades. Yet many of those Earth-sized planets are only characterized in mass and radius. Therefore, interior structure models rely heavily on equations of states (EOS) for rock material to characterize the planetary properties. One particular interesting material is iron oxide, which is very challenging to treat with standard Density Functional Theory (DFT) methods. Here we investigate the DFT+U approach to obtain the correct electronic and structural properties for the FeO phases typically predicted at the high pressures within the planetary interiors. The Hubbard U is obtained self-consistently from spin-polarized DFT calculations with QUANTUM ESPRESSO [1,2] using the linear response approach [3]. The resulting optimized ground state is used as a starting point for phonon calculations within the quasi-harmonic approximation. Based on these calculations we investigate the impact of the Hubbard U on the EOS providing a step forward to incorporating more realistic rock material into interior structure models of super-Earths.

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Ionization Potential Depression inWarm Dense Matter studied with Ab Initio Simulations

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The effect of Ionization Potential Depression (IPD) plays an important role in accurately describing the electronic and optical properties of materials in the Warm Dense Matter (WDM) regime, which is characterized by a degeneracy $\Theta \approx 1$ as well as a coupling parameter $\Gamma \approx 1$. Recent experiments have shown that the widely used models to describe IPD, like Stewart and Pyatt (SP) or Ecker-Kröll do not reproduce experimental results to a satisfying degree. This is especially the case in the high-density regime, which wasn't experimentally accessible until recently. In this work we thus investigate IPD by using ab initio DFT/DFT-MD simulations for carbon, aluminum, argon and iron. We compare our findings to the IPD description of the SP model. The comparison shows a large discrepancy between both approaches. One of the underlying assumptions of the SP model is that electronic states are always elevated into the continuum when they reach an eigenenergy ≥ 0. Our ab initio simulations disagree with this assumption and do not reproduce such behavior. We show that the state with eigenenergy 0 and a uniform probability distribution in the bulk, which is assumed to always exist in the SP model, cannot be produced in our simulations for aluminum. Thus, we advice the reader to be careful when using SP for experimental interpretations. Our approach furthermore shows that older models do not account for many-particle effects correctly in the high-density regime.

X-ray microscopy in High Pressure Research at the ID15B beamline

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Nowadays high pressure (HP) research is one of the popular scientific directions. In combination with other extreme environments (magnetic field, temperature) it allows scientists to discover the new properties of the materials, improve their phase diagrams, and simulate the conditions in the interior of planets. First beamlines for HP research were oriented generally to the X-ray diffraction (XRD) and X-ray scattering. For X-ray focusing, Bragg-Fresnel optics and mirrors [1] were used. In this paper we want to present the refurbished in-line refractive optics [2] based ID15B beamline at the ESRF [3]. The experience of the refractive optics implementation in HP research at the ID06 [4] served as a basis for the beamline designing. ID15B is oriented to the XRD and X-ray microscopy experiments. The significant advantage of this beamline is that, with almost the same set up (i.e. without moving Diamond Anvil Cell (DAC) and lasers), we can collect X-ray diffraction, probe the phase composition of the samples, and then record high resolution X-ray images checking any phase transitions or chemical reactions. X-ray radiation is produced by canted undulator with source size 30 x 125 mm (V x H). For X-ray focusing on the spot with the same vertical and horizontal sizes on the sample placed at 44 m from the source, the two transfocators are used. They are placed on both sides of the monochromator in a white and monochromatic beam (34 m and 42 m from the undulator) and equipped with linear compound refractive lenses manufactured from Be and have 200 mm radii of curvature of the parabola profiles. X-ray beam energy on the beamline is fixed to 30 keV by cryogenically cooled Si (111) single crystal monochromator with horizontal deflection that is located at 35 m from the undulator source. The flat panel detector MAR555 for XRD is placed on the same stage with the X-ray objective that makes it easy to switch between XRD and X-ray microscopy. X-ray objective consists of Be and Al two-dimensional refractive lenses with 50 mm radii of curvature of the rotated parabola profiles. The sample image transmitted by these lenses is recorded by PCO CCD camera with 0.74 mm pixel size that is placed 5 m from the sample stage.

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Thermal conductivity of water plasmas from ab initio simulations

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The determination of thermal conductivities of dense plasmas is a great challenge for both experimental and theoretical approaches. In partially ionized plasmas, not only electrons contribute to the thermal conductivity but also ions. Here we use ab initio molecular dynamics (MD) simulations based on density functional theory (DFT) to calculate the ionic contribution to the thermal conductivity of dense partially ionized water plasmas [1]. The required heat current of the ions is determined by matching the forces from each of the DFT-MD simulations onto effective pair interaction force fields. These force fields are then used to evaluate the Green-Kubo relation for the thermal conductivity using the ion trajectories of the same DFT-MD simulation run. This approach is generally applicable to various multi-component plasmas as well as to materials in liquid, solid, or superionic phases. For water plasmas, the ionic contribution to the thermal conductivity is found to be equal to or greater than the electronic contribution [2] up to temperatures of 20 000 K, depending on the density. The presence of characteristic contributions from thermal dissociation reactions of the water molecules can be traced back to the shapes of the derived force fields between the ionic species. These contributions enhance the ionic thermal conductivity between 3000 and 10 000 K noticeably and are more pronounced toward low densities. Additional benchmark calculations for ice VII and liquid water show good agreement with experimental data and with an ab initio study in which the ionic heat current was determined with a generalized variant of density functional perturbation theory for the electronic ground state [3]. Our results [1] are of general significance for understanding thermal transport properties in dense, partially ionized plasmas and other states of matter. The generated thermal conductivity data for water are particularly important for the development of non-adiabatic evolution models for water-rich giant planets like Uranus and Neptune.

This work is supported by the DFG within the FOR 2440 “Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics.”

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X-ray diffraction studies of materials laser-heated in double stage diamond anvil cells

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In the first part of this work, we report in situ X-ray diffraction study of RexCy compounds formed as result of chemical interaction between secondary diamond anvil and rhenium gasket during pulsed laser heating of double stage diamond anvil cells (dsDACs) made of nanocrystalline diamond (NCD) semispheres. Several high pressure polymorphs of rhenium carbides, such as, hexagonal Re2C, anti-B8-type structured ReC0.2, WC-type structured ReC, and orthorhombic ReC2 have been observed at pressures ˜200 GPa. Diffraction experiments were conducted at the nanoprobe beamline ID11 at the European Synchrotron Radiation Facility, Grenoble, France (Frelon4M detector, l = 0.30996 Å, beam size 0.45*0.45 μmˆ2 at FWHM). The second part of my report dedicated to test capabilities of secondary anvils shaped with focused ion beam (FIB). In combination with nano-beam setup at extreme condition beamline P02.2 at Petra III, DESY, Hamburg, Germany (Perkin Elmer XRD1621 flat panel detector, l=0.4853 Å, beam size 0.7*0.8 μmˆ2 at FWHM) we tested several secondary stage diamond anvils of different shape (cones (10-20 μm), beveled anvils (8° slope cut), toroidal), prepared with FIB from single crystal diamond plate. We found that yield strength of such anvils could reach about 400 GPa at confinement pressure of about 70 GPa and peak pressure over 220 GPa.

Paramagnetic-to-diamagnetic transition in dense liquid iron and its influence on electronic transport properties

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The electronic transport properties of warm dense liquid iron are important properties for understanding the magnetic field generation in Earth-like and other solid planets. Here we investigate the electrical and thermal conductivity with spin-polarized simulations based on density functional theory over a significant pressure and temperature range using the Kubo-Greenwood formalism [1]. We find that a paramagnetic state is stable in the liquid up to high temperatures at ambient pressure. It is shown that the overestimation of results from exploding wire experiments by more than 30% that occurs in spin-degenerate simulations is reduced to 10% or less when spin polarization is taken into account. Direct comparisons between spin-polarized and spin-degenerate simulations reveal that the spin effects on the conductivities enter via changes in both ionic and electronic structure. Along the 3700 K isotherm, we explore the persistence of magnetic fluctuations toward high densities, and beyond 20-50 GPa the liquid becomes diamagnetic, which suggests the existence of a continuous paramagnetic-to-diamagnetic transition. This transition exerts a significant influence on the transport properties of liquid iron and is potentially of high relevance for dynamo processes in Mercury and Mars.

This work is supported by the DFG within the FOR 2440 “Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics.”

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Hydrogen in the Earth's core

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Water plays many critical roles in Earth dynamics and the rise of life. Furthermore, the origin, concentration and distribution of water in the Earth is key for our understanding of the current Earth and its history, as water has profound influences on the Earth's seismic and physico-chemical properties that regulate differentiation processes, plate tectonics, volcanism and geochemical reactions[1,2]. Current estimates of the budget and distribution of water in the Earth have large uncertainties, most of which come from the lack of information about the deep Earth[1]. Recent studies suggest that the Earth could have gained a considerable amount of water during the early stages of Earth's evolution from the hydrogen-rich solar nebula, and that most of the water in the Earth may have partitioned into the core[2-4]. Here, we calculate the partitioning of water between iron and silicate melts at 20-135 gigapascals and 2800-5000 kelvin, using *ab initio* molecular dynamics and thermodynamic integration techniques. Our results indicate a siderophile nature of water at oxidizing condition ($P_{H_2O}/P_{H_2+H_2O}$=1), which will be weakened with the increasing reducing conditions and increasing temperature; nevertheless, hydrogen always partitions strongly into the iron liquid. The siderophile nature of hydrogen is also verified by an empirical counting method which sees the distribution of hydrogen in an equilibrated iron and silicate melt. We therefore conclude that the Earth's core can act as a large reservoir of water. The findings can further constrain Earth accretion models and water distribution, and may also account for the mismatch between mineral physics and seismic observations in the Earth's outer core.

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Constraining the rotation period of Saturn and Neptune with the Love number k2

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The rotation periods of Saturn, Uranus, and Neptune are not well known. Estimates for Saturn include 10h 32m derived from minimization of wind velocities and dynamical heights [1], 10h 33.5m using ring oscillations [2], as well as 10h 39m and 10h 47m derived from Voyager and Cassini magnetic field observations, respectively [3]. For Neptune, the wind velocity and dynamical height minimization methods predict a 1h 21m longer period than the Voyager magnetic field observations [4]. Here I present the static contribution to the Love number k2 of interior models of Saturn and Neptune for different rotation rates. For Neptune, a strong enhancement in k2 by 15% has been found [5], from 0.424 to 0.495, upon increasing the rotation period by 1h 21m. The same approach presented in [5] for the Neptune-Triton system is applied in this work to Saturn. Although k2 may be influenced in addition by dynamical effects, if those are comparably small I suggest that observational determination of k2 by an orbiting spacecraft may be used to better constrain the planets' rotation.

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The Melting Line and the Band Gap of Helium from First Principles Simulations

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We studied the behavior of solid and liquid helium under high pressure with molecular dynamics simulations based on density functional theory (DFT-MD). Helium, as the second most abundant element in nature, is important for astrophysical applications, e.g., the modeling of the interior and evolution of gas giants and brown dwarfs. In particular, we calculated the melting line and examined the insulator-to-metal transition at extreme pressures up to the TPa region. The calculation of the melting line is a challenging topic in computational physics. Out of many approaches of different complexity and efficiency, two-phase simulations represent a very intuitive approach with high accuracy. We have implemented this method and investigated finite-size effects, as well as the convergence of other parameters. We found good consistency with available experiments and gave predictions for the melting line of helium up to the TPa region [1]. Laser-driven compression experiments have shown that helium undergoes an insulator-to-metal transition at high density and temperature [2]. However, the exact location and nature of this transition is not clear yet. The most recent publications on the calculation of the helium band gap closure [3, 4] differ within a factor of two in density and employ different definitions of the band gap. We performed extensive convergence tests and our preliminary results are in good agreement with the results of Zhang et al. [3]. We will continue to calculate the band gap closure, as well as the EOS, the DC conductivity, and the optical reflectivity in the regime where the helium band gap closes.

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Shock compression of SiO2 and its analogues at megabar pressures

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SiO2 is one of the most fundamental constituents in planetary science, being vastly abundant in the Earth's crust and mantle. As an essential 'building block', it bonds with Mg, Fe and other elements to form major mineral phases and even free SiO2 can be expected in localized regions in the Earth's mantle, derived from e.g. subducted oceanic crust [1]. The stability of SiO2 within these regions is affected by polymorphism at high pressures and SiO2 serves as an archetype for the dense highly coordinated silicates of planetary interiors and large (1-10 M_Earth) exoplanets [2]. Seismological heterogeneities in the ultralow velocity zones (ULVZs) at the upper end of the transition zone and at the core mantle boundary (CMB) have been interpreted with the presence of higher coordinated SiO2 melts [3,4]. The possible presence of silicate melts may result from partial melting of the lowermost mantle minerals or are remnants of the dense basal magma ocean [5], however, up to date it is only little known about these SiO2 melts within the field of geosciences. We carried out time-resolved X-ray diffraction studies of quartz, fused silica, stishovite and GeO2 at megabar pressures, using the long-pulse laser and shock diagnostics at the MEC end-station of the Linac Coherent Light Source (LCLS), USA. Our study mainly focused on the in-situ investigation and determination of Si/Ge-O bond length during shock compression, and consequently, its structure factors and radial distribution. Due to its recent upgrade, the ns-laser at MEC allowed us to compress fused silica, quartz and GeO2 to pressures of up to 140 GPa following their respective Hugoniot and reaching temperatures corresponding to the SiO2/GeO2-liquidus regime. Stishovite was driven to the high-pressure CaCl2-, PbO2- and pyrite structures (rho_max = 6.46 g/cm3). While simultaneously probing the samples with highly resolved X-ray diffraction at various time delays, it was possible to obtain time-resolved information of the lattice structure during phase transitions, melting and re-crystallization.

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Nanodiamonds from laser-induced shock compression of polystyrene – extraction under way

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In previous experiments with high intensity laser the production of nanodiamonds from different hydrocarbon precursors was demonstrated using in situ femtosecond X-ray diffraction with an XFEL. During the nanosecond experiments in the laboratory planetary interior conditions comparable to that of Uranus and Neptune (˜5000K, ˜150GPa) are reached. Thus, a similar phase separation of hydrocarbons into hydrogen and carbon can be expected within the ice giants. Interestingly, under these warm dense matter conditions hydrogen is predicted to be metallic and consequently may drive the nucleation of diamonds that presumably precipitate towards the planetary centre. Since the nanodiamond formation process from hydrocarbons is not fully understood yet, high speed recordings were collected to gain insights into the kinetics. In addition, a recovery set-up offered the possibility for potential post-analysis. Analogous to NASA's Stardust mission highly porous SiO2 and other inorganic aerogels along with solid Cu plates served as catcher media. The challenge is to successfully recover a very low amount of nanoparticles. We know that the particle size is around 4nm and that 60% of the carbon atoms in polystyrene (CH) are transferred into a diamond lattice. However, with a focal spot of 500µm and a 125nm thick polystyrene foil the total yield is ˜16µg of nanodiamond material along with other remaining hydrocarbons and graphite from the warm dense matter mixture. Fairly aggressive chemicals (e.g. HF, HNO3, H2SO4, HClO4) under elevated temperatures and pressures are typically used to isolate, purify and concentrate nanodiamonds for example from detonation soot or meteorites. The goal is the application of an efficient chemical procedure along with precise sample handling to collect enough material to be above the detection limit for the post-analysis instruments (Raman, XRD, SEM, TEM). The poster presents the most recent data obtained in the framework of the nanodiamond project and gives an outlook of further steps necessary for an unambiguous identification followed by a thorough characterisation. This work holds crucial implications for planetary interior models as well as a potential alternative for a further industrial production technique of nanodiamonds.

Laser wakefield accelerated betatron beam for absorption spectroscopy of ultrafast Warm Dense Matter

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We present a platform to study ultrafast heating of Warm Dense Cu diagnosed by the means of x-ray absorption spectroscopy to be carried at Draco laser at HZDR. A thin Cu foil is heated to few eV temperature either directly by a laser or by laser-generated proton beam and probed with variable delay by a laser-driven betatron radiation. This betatron radiation, emitted by laser wakefield accelerated electrons, is a unique x-ray source with its ultrashort duration and broadband spectrum, therefore it is ideally suited for studies of non-equilibrium dense plasmas. The sample is studied via the X-ray Absorption Near Edge Spectroscopy (XANES) in region above the Cu K-edge at 8.9 keV. This method provides temporally-resolved information about both the ionic structure of the matter and its temperature during the process of ultrafast heating and melting of the material. We deployed a newly developed spectrometer with a highly reflective HOPG crystal in a geometry well suited for detection of low intensity signals with high spectral and angular resolution.

Simulations of warm dense C-H mixtures

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The thermodynamics of warm dense CH mixtures are important for the description of astrophysical objects and for a number of technical applications. We have calculated the thermodynamic functions and mixing properties, as well as other quantities for CH mixtures at three different conditions as created in recent experiments. For one of these conditions, demixing of C and H was observed. We discuss how and why the DFT-MD simulations correctly predict or fail to predict these processes.