# HP4 2017 Max-Planck-Campus Göttingen Oct. 4-6



# 6th workshop on High Pressure, Planetary and Plasma Physics

# Abstracts

# HP4 Program

#### 13:30 Welcoming **Session 1: Exoplanets** 13:40 RAINERS, ANSGAR Invited talk p. 7 What do we know about exoplanets? CSIZMADIA, SZILARD 14:20 p. 7 Love-number determinations for exoplanets from transit light curves SOHL, FRANK 14:40 p. 8 How does the B1-B2 phase transition of ferropericlase (Mg,Fe)O affect the light curve of a transiting super-Earth-type planet? p. 9 15:00 **KELLERMANN**, CLEMENS Interior structure models and fluid Love numbers of exoplanets in the super-Earth regime 15:20 WAGNER, FRANK p. 10 Geochemical cycling of greenhouse gases between interior and atmosphere 15:40 **Coffee & posters Session 2: Experiments I** 16:10 SMITH, RAYMOND Invited talk p. 11 High-pressure X-ray diffraction measurements over picosecond timescales on the Stanford Linac Coherent Light Source (LCLS) and the Dynamic Compression Sector (DCS) 16:50 APPEL, KAREN p. 12 Perspectives for dynamic and static high pressure research at the High Energy Density science instrument at European XFEL 17:10 SCHÖLMERICH, MARKUS p. 14 Dynamic compression experiments with the new High Energy Density Science (HED) instrument at the European XFEL 17:30 **Poster session (with beer & wine)**

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12:10	HELLARD, HUGO Tidal response of the ice-ocean system on Enceladus	p. 20
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13:50	CARACAS, RAZVAN Invited talk Supercritical silicate melts during and in the aftermath of the Giant Impact	p.21
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16:40	HARTLEY, NICHOLAS Hydrocarbons at Extreme Conditions	p. 27
17:00	SAN JOSÉ MÉNDEZ, ALBA Fast X-ray diffraction of (MgFe)O across the spin transition under dynamic compression	p. 28
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09:40	BRADBY, JODIEInvited talkFormation of Metastable Phases of Silicon and Germanium	p. 30
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# WHAT DO WE KNOW ABOUT EXOPLANETS? Rainers, Ansgar

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Astronomical exoplanet research has matured from discovery to characterization mode. We know of several thousand exoplanets that exists around other stars, and many of them can be studied with complementary methods. This has provided a wealth of information about planetary systems, and it has shown us a rich diversity of objects for which physical models of formation and structure are required. I will give an overview about conclusions relevant for our understanding of exoplanet interiors and how we expect the astronomical landscape to evolve.

# LOVE-NUMBER DETERMINATIONS FOR EXOPLANETS FROM TRANSIT LIGHT CURVES

# Csizmadia, Szilard

Institut for Planetary Research, DLR, Berlin, Germany

Masses, radii and thus mean densities of exoplanets are routinely determined from combined radial velocity and transit light curve analyses. However, these three parameters are not enough to fully constrain the composition and the interior of an exoplanet in every case because the mass-radius diagram shows degeneracies (e.g. Wagner et al. 2011) as well as the mass-density diagram shows a remarkable diversity in the small mass regime (e.g. Hatzes and Rauer 2015). A natural choice of a third parameter which may break down these degeneracies is the fluid Lovenumber of an exoplanet. This can be determined from orbital decay or it may be estimated from the shape of the exoplanet. In this talk I review the methodology of Love-number measurements in case of out-of solar system objects and I mention the already published results. I also introduce our code and the improvements we plan to include for measuring the exoplanetary shape. A case study is shown how precisely one can determine the shape when we assume realistic photometric noise levels.

## How does the B1-B2 phase transition of ferropericlase (Mg,Fe)O affect the light curve of a transiting super-Earth-type planet?

# Sohl, Frank

Institut for Planetary Research, DLR, Berlin, Germany

The characterization of solid exoplanets in terms of internal structure and atmospheric composition is important to understand their formation, orbital evolution, and possible habitability. Structural models of low-mass solid planets of less than ten Earth masses are created by using equations of state valid in the high pressure limit for the radial density distribution [1]. Successful models that satisfy the observed planetary radius and mass still suffer from model ambiguities, mainly due to the imperfect knowledge of the internal mass distribution and the possible existence of pressure-induced phase transformations. To partly overcome these limitations, rotationally and tidally induced planetary shape determinations have been invoked as additional model constraints for the concentration of mass toward the center [2]. We here consider structural models of a generic transiting super-Earth planet (6 Earth masses, 1.75 Earth radii), subdivided into an iron core overlain by an MgO-rich mantle, and calculate corresponding shape parameters and light curve variations based on determinations of the secular or fluid Love number  $k_{2,f}$ . In particular, we are interested in the sensitivity of  $k_{2,f}$  to the structural phase transition from the cubic B1 (NaCl-type) structure to the B2 (CsCltype) phase of ferropericlase (Mg,Fe)O at mantle pressures above 500 GPa [3], corresponding to a depth of about 4500 km. However, our preliminary calculations suggest that the incorporation of the structural phase transformation in these models does not substantially affect  $k_{2,f}$  since only the lower 1/5 of the total mantle volume would be affected by the relatively small density contrast between the B1 structure and the B2 phase. Consequently, the effect on  $k_{2,f}$  would be more pronounced for more massive planets with smaller or even non-existent cores. We will discuss implications for corresponding shape determinations and astronomical light curve variations.

References:

[1] Wagner, F.W. et al.: Interior structure models of solid exoplanets using material laws in the infinite pressure limit, Icarus 214: 366-376, 2011.

[2] Correia, A.C.M. and Rodriguez, A.: On the equilibrium figure of close-in planets and satellites, Astrophys. J. 767:128 (5pp), 2013.

[3] Cebulla, D. and Redmer, R.: Ab initio simulations of MgO under extreme conditions, Phys. Rev. B 89, 134107, 2014.

#### INTERIOR STRUCTURE MODELS AND FLUID LOVE NUMBERS OF EXOPLANETS IN THE SUPER-EARTH REGIME

# Kellermann, Clemens

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The increasing number of discovered exoplanets provides us with new planetary classes, such as super-Earths and mini-Neptunes. In order to model their interior structure the mean density of a planet is an important input. Based on this quantity we can decide whether extensive gaseous layers or rocky mantle materials have to be considered. In this work we calculate three-layer models with an adiabatic outer layer of volatile material and isothermal, solid inner mantle (MgO) and core (Fe) as well as the resulting Love numbers  $k_2$ . This quantity results from the planet's internal density profile and, if also measured, can be used to constrain the possible layer compositions and sizes. To examine the effect of planet mass, layer sizes and surface temperature on internal structure and Love number we perform a parameter study. Furthermore, we apply the results to analyze several known exoplanets with measured densities in the regime of super-Earths and mini-Neptunes. We find that an observational constraint on  $k_2$  would be particularly useful to narrow down the planetary Fe/MgO mass ratio.

# GEOCHEMICAL CYCLING OF GREENHOUSE GASES BETWEEN INTERIOR AND ATMOSPHERE

# Wagner, Frank

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Although geochemical cycling is of fundamental importance to processes such as climate variability, the history of volatile fluxes between interior and atmosphere remain controversial. Therefore, we examine in this study the geophysical factors that regulate the atmospheric abundances of H2O, CO2, and N2. Our modelling approach includes a fully dynamical convection simulation, the transport of volatiles into and out of the convecting mantle, and a varying surface temperature due to infrared absorption in the atmosphere. We have linked these processes to compute simultaneously the thermal evolution of atmosphere and mantle. Depending on model parameters (e.g., critical yield strength, reference viscosity, solar insolation), the evolving planet passes through episodic and plate tectonic regimes. Planets with plate tectonics possess a mobile surface over extended periods of time. With respect to our simulations, we find an average plate speed ranging between few to several tens of cm/yr, which is slightly higher than what is observed on presentday Earth. Plate tectonics leads to efficient cooling of the interior and a well mixed mantle. Melt production and volcanism ensure the release of volatiles from the interior into the atmosphere at a constant rate. The excess amount of greenhouse gases is continuously removed from the atmosphere by weathering processes of the geochemical cycles, thus keeping variations in surface temperature under control. Furthermore, the formation of cratons on planets with plate tectonics stabilises the amount of rocks exposed to chemical weathering and dampens short-term fluctuations in the surface temperature. Planets with episodic tectonics show periods of quiescence punctuated with rapid episodes of surface overturn. Our simulations suggest that catastrophic resurfacing occurs randomly and takes place over about 50 Myr. During such global-scale overturn events, the average plate speed reaches high values of a few hundreds of cm/yr. In comparison to the plate tectonic regime, planets with episodic resurfacing show a different cooling history and mantle mixing. Because of elevated melt production and volcanism, catastrophic resurfacing causes strong variations in surface temperature on the order of a few tens of Kelvin, which could be enough to push a planet into greenhouse runaway. The characteristic differences between the two tectonic regimes may explain the divergent evolution of Venus and Earth as suggested by previous studies (e.g., L. Noack et al. (2012) and C. Gillmann & P. Tackley (2014)).

## HIGH-PRESSURE X RAY DIFFRACTION MEASUREMENTS OVER PICOSECOND TIMESCALES ON THE STANFORD LINAC COHERENT LIGHT SOURCE (LCLS) AND THE DYNAMIC COMPRESSION SECTOR (DCS)

# Smith, Raymond

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Experiments on the Materials at Extreme Compression (MEC) beamline at the Stanford Linac Coherent Light Source (LCLS) and the Dynamic Compression Sector (DCS), couple high power laser drivers with monochromatic x-rays to obtain high signal-to-noise diffraction patterns from shock- or ramp-compressed samples to pressures above 200 GPa. The LCLS delivers monochromatic photon energies ( $\Delta E/E \sim 2 \times 10^{-3}$ ) tunable over 0.27-11 keV range (1st harmonic) within a 5-500 fs pulse and with up to 2 mJ of energy (1012-1013 photons/pulse). Samples are dynamically compressed with a high-power laser driver which delivers up to 70 J in a 15 ns pulse. Laser pulse shaping capabilities permit control of the thermodynamic compression path and the compression rate within a material undergoing a phase transformation. LCLS can operate up to 120 Hz or, as is typical for the x-ray diffraction experiments described here, in single shot mode. The LCLS-II upgrade in FY19 will extend the x-ray energy to 25 keV and further increase the options for high-pressure diagnosis of phase transformation kinetics. Here we present data on high-pressure phase transformations in SiC and Zr compressed over nanosecond timescales – with evidence of kinetic effects at these rapid compression timescales. Details of similar experiments at the Dynamic Compression Sector located at the APS will also be discussed.

## PERSPECTIVES FOR DYNAMIC AND STATIC HIGH PRESSURE RESEARCH AT THE HIGH ENERGY DENSITY SCIENCE INSTRUMENT AT EUROPEAN XFEL

# Appel, Karen

European XFEL, Schenefeld, Germany

Recent developments in high-pressure techniques have significantly enlarged the possibilities of experimental planetary research: with the development of doublestage Diamond Anvil Cells (DACs), the structure of matter can now be studied statically at pressures beyond 1 TPa [1]. In addition to static conditions, more and more extreme conditions can be achieved by fast drivers such as dynamically driven DACs, laser shocks or pulsed-laser heated DACs. While the first two drivers enable measurements of pressure-induced phase transformations at different strain rates, the latter allows to study the properties of matter at extreme PT conditions. With the increase in pressure, experimental challenges grow since stable conditions are either extremely short-lived or small in size.

A high number of X-ray photons per pulse and short pulse lengths are vital to obtain structural information on time scales of fast phase transitions. European XFEL, in Schenefeld, Germany is the first FEL in the hard X-ray regime. It will produce about 1012 photons/pulse in the energy range between 5 and 25 keV at maximum repetition rates of 4.5 MHz. Due to the availability of the high photon energies and its high brilliance which allows focusing to below the Âţm scale, it will be the first FEL enabling XRD studies in DACs.

The High Energy Density science instrument (HED) [2], one of the six baseline instrument stations at European XFEL, is dedicated for research at extreme conditions and will also offer the possibility of static and dynamic compression experiments at pressures above 100 GPa [3,4]. The Helmholtz International Beamline of Extreme Fields (HIBEF) will contribute key-instrumentation to HED that enables to reach extreme conditions [5]. In addition to DAC experiments, it will be feasible to perform dynamic compression experiments or using high-energy optical lasers (100 kHz/40 mJ/ps or 10 Hz/100J/ns).

In this contribution we give an overview of the capabilities of the future HED science instrument with respect to expected X-ray beam properties and how these can be exploited for high-pressure experiments. HED will be available for users from 2018 on.

[1] Dubrovinskaia N. et al. (2016) Materials Science, 2(7), e1600341. http://doi.org/10.1126/sciadv.1600341 [2] www.xfel.eu/research/instruments/hed

[3] M. Nakatsutsumi et al., Technical design report: Scientific instrument High Energy Density Physics (HED), XFEL:EU TR-2014-001, Germany, 196 p (2014). doi:10.3204/XFEL.EU/TR-2014-001.

[4] K. Appel et al., Plasma Phys. Control. Fusion 57, 014003 (2015).[5] www.hibef.de

# DYNAMIC COMPRESSION EXPERIMENTS WITH THE NEW HIGH ENERGY DENSITY SCIENCE (HED) INSTRUMENT AT THE EUROPEAN XFEL

# Schölmerich, Markus

European XFEL, Schenefeld, Germany

With the discovery of more than 3600 exoplanets in the past twenty years, the understanding of compositional and structural properties of large ( $\sim$ 1-10 M<sub> $\oplus$ </sub>) rocky planets has gained great interest. For instance, precise knowledge on the equation of state and the high-pressure phase diagram of the planetary materials is needed to construct interior, evolution and dynamo models. The use of the new experimental facility, the High-Energy Density Science (HED) instrument at the European XFEL will allow to investigate matter at extreme conditions by laser induced shock- and ramp compression [1, 2]. It will be possible to investigate the model system MgO at pressures of up to 1 TPa and several 1000 K with the temporal pulse shaping capability of the optical long pulse laser DIPOLE100X, which will allow quasiisentropic compression of material, reaching off-Hugoniot high pressure states. These short-lived states will be investigated with various Xray diagnostic tools such as XRD, XANES and IXS. Sample design will consist of polycrystal MgO to be deposited as successive coatings directly on a pressure window (LiF). Typical thickness of the sample will be varying from a few  $\mu$ m up to a maximum of 20  $\mu$ m - depending on the desired spatial pressure distribution. Specific heating procedures during the process of deposition will enhance the XRD signal. Experimental results will be compared to ab initio simulations to benchmark experimental key phases at the relevant conditions [3]. Ultimately, we are going to obtain equation-of-state (EOS) data for MgO including its melting curve. First simulations with the plasma hydrodynamics code ESTHER [4] revealed experimental conditions, in which peak pressures of more than 7 Mbar and temperatures between 4000 and 6000 K were achieved - equivalent to those of middle- and lower mantle conditions within exoplanets. References

[1] Appel, K., Nakatsutsumi, M., Pelka, A., Priebe, G., Thorpe, I. and Tschentscher, T. (2014) Studying planetary material using intense x-ray pulses. Plasma Phys. Control. Fusion 57(1), 014003.

[2] Tschentscher, T, Bressler, C., GrulLnert, J., Madsen, A., Mancuso, A.P., Meyer, M., Scherz, A., Sinn, H. and Zastrau, U. (2017) Photon Beam Transport and Scientific Instrument at the European XFEL. Applied sciences 7(6), 592.

[3] Cebulla, D. and Redmer, R. (2014) Ab initio simulations of MgO under extreme conditions. Phys. Rev. B, 89(13), 134107.

[4] Colombier, J.P., Combis, P., Bonneau, F., Le Harzic, R., Audouard, E. (2005) Hydrodynamic simulations 14

# HIGH PRESSURE AND HIGH TEMPERATURE PHASE DIAGRAM OF AMMONIA MONOHYDRATE

# Ninet, Sandra

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Knowing the properties of H2O, NH3 and their mixtures under high pressure and temperature is important for planetary science because these H-bonded ices are present in Jovian planets and their satellites under a wide range of pressure (P) and temperature (T) conditions. The high P-T properties of the pure ice compounds have been the focus of many investigations, which have revealed a rich polymorphism. By contrast with the pure components, there are rather few information available on the properties of the dense phases of H2O/NH3 mixtures, although the latter are crucial for the description of icy planets.

Depending on the mixture concentration, three types of ammonia/water compounds can be obtained: ammonia monohydrate (H2O,NH3) (noted AMH), ammonia hemihydrate (H2O,2NH3) and ammonia dihydrate (2H2O,NH3). Experimental high-pressure studies on AMH have been done up to 10 GPa and six phases have been reported. The structure of phase VI [1] is of particular interest as it is a substitutionally-disordered molecular alloy whose simple bcc structure is related to that of H2O ice VII. A theoretical study [2] has suggested that the ammonia monohydrate (AMH) molecular solid transforms into an ionic solid composed of NH4+ and OH- ions, in a similar fashion as the self-ionization observed in pure ammonia [3,4], but at much lower pressures (10 GPa instead of 150 GPa), thus much easier to reach in experiments.

In this presentation, we will present new experimental and theoritical investigations of the phase diagram of AMH. In particular, to test this surprising prediction, we have performed infrared absorption studies, Raman scattering and Xray/neutrons diffraction of AMH up to 40 GPa. We will discuss the existence of the molecular/ionic phase transition. We will also present our recent experimental results on the phase diagram of AMH at high pressure (40 GPa) and high temperature (700 K).

[1] J. S. Loveday and R. J. Nelmes, Phys. Rev. Lett. 83, 4329 (1999)

[2] G. I. G. Griffiths, A. J. Misquitta, A. D. Fortes, C. J. Pickard, and R. J. Needs, J. Chem. Phys. 137, 64506 (2012)

[3] S. Ninet, F. Datchi, P. Dumas, M. Mezouar, G. Garbarino, A. Mafety, C.J. Pickard, R.J. Needs and A.M. Saitta, Phys. Rev. B, 89, 174103 (2014)

[4] T. Palasyuk, I. Troyan, M. Eremets, V. Drozd, S. Medvedev, P. Zalesky-Ejgierd, E. Magos-Palasyuk, H. Wang, S. Bonev, D. Dudenko et P. Naumov, Nat. Comm., 5, 3460 (2014)

# THERMAL EVOLUTION AND CORE STRATIFICATION OF MERCURY **Rivoldini, Attilio**

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Like the Earth, Mercury has a global magnetic field that is powered by convective motions in its liquid iron-rich core. Convective motions are mainly generated by iron-alloy crystallization, light element exsolution, and secular cooling. Thermal evolution studies indicate that the present-day heat flow at the core mantle bound-ary of Mercury is subadiabatic. As a consequence a stable thermal boundary layer could form at the top of its core. Additionally, the formation of iron-rich snow and chemical reactions between the mantle and the core could lead to the formation of a chemically stable layer in the core. A stable upper core thermally conductive layer reduces the core cooling rate, affects the inner core evolution, and the dynamo action. In this study, we use a coupled thermal evolution model of the core and mantle to constrain the interior structure of Mercury. We assess conditions for the formation of a stable stratified layer in the core and study how it affects the evolution of the inner core and core dynamo action.

# The thermal evolution of Mercury's Fe-Si core

# Knibbe, Jurrien

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We present results of thermal evolution study with a core of Fe-Si. Si does not significantly fractionate between liquid and solid metal, such that solidifying a core of Fe-Si alloy does not produce compositional convection (Kuwayama and Hirose, 2004). Because compositional convection (that would be produced by solidifying a core from Fe-S composition for example) would penetrate the thermally stratified upper core layer (Manglik et al., 2010), the Fe-Si core is consistent with the proposed stably stratified layer in the outer part of the core as explanation for Mercury's low magnetic field strength and broad scale geometry (Christensen 2006). Other characteristics of an Fe-Si alloy are an increased release of latent heat upon core solidification, a reduced thermal conductivity, and a lowered melting temperature compared to pure Fe. We have adopted a conductive temperature profile in the region of the core that has a subadiabatic heat flow, consistent with the expected thermal behavior. This introduces a flexibility in the model such that temperature variations in the core relax when the CMB heat flow drops. As a result, higher outer core and mantle temperatures are achieved, facilitating a partially liquid Fe-Si outer core. Also, the deeper core region cools independent of the temperature evolution at the CMB, which results in a more gradual core growth and makes a magnetic field generation of Mercury throughout its evolution possible. Also, the increased latent heat of Fe-Si metal boosts the dissipative energy required to drive a dynamo, while the upper liquid core layer remains stably stratified in absence of compositional convection.

# BASIN-SPECIFIC CONSTRAINTS ON THE THERMAL EVOLUTION OF THE TERRESTRIAL PLANETS

# Padovan, Sebastiano

DLR, Berlin, Germany

The surfaces of Mercury, the Moon, and Mars are largely the results of interior processes that operated over the age of the solar system. These surfaces are also the location of copious amounts of data (e.g., imaging and spectrometry over a wide range of wavelengths). However, it is not straightforward to connect these surficial datasets, however abundant, to the interior processes that ultimately are the cause of the observed data. The only direct constraints available when investigating the interior evolution of the terrestrial planets are related to the nature (volcanic/primordial), volume, and age of their crusts. In this work we start by investigating numerical models for the thermal evolution of Mercury consistent with the properties of their crusts. In addition, we include the geodynamical effects of large impacts on the interior evolution. We focus on reproducing the inferred volume and time of emplacement of the volcanic infillings associated with the large impact basins Caloris and Rembrandt. This novel approach has the advantage of combining the few global constraints provided by the properties of the crust with the local datasets relative to the large impact basins. We test and validate the method on Mercury, where we can properly reproduce the observed physical and spectral properties of its large basins. We conclude providing an outlook for the application of the method to the Moon and Mars.

#### VIBRATIONAL AND THERMODYNAMIC PROPERTIES OF MATERIALS AT HIGH PRESSURE AND HIGH TEMPERATURE FROM AB-INITIO MOLECULAR DYNAMICS

# **Bouchet**, Johann

CEA, Arpajon, France

Usually, thermal vibrations of atoms can be taken into account via the so-called quasiharmonic approximation (QHA). In this framework, the phonon dispersion relations are calculated at 0 K using density functional perturbation theory (DFPT) and the temperature is included only via the thermal dilatation, i.e., by computing the phonon spectrum at different volumes. The main drawback of this approximation is that its accuracy is difficult to assess since anharmonic contributions beyond quasiharmonicity are difficult to estimate. But if the harmonic part of the atomic vibrations dominate the free energy at elevated temperatures, the neglect or an inaccurate evaluation of seemingly minor contribution as the anharmonic one can result in falsely predicted phase stabilities or inaccurate phase transition temperatures. Here we will present a recent method, called the temperature dependent energy potential (TDEP) that provides a consistent way to extract the best possible harmonic (or higher order) potential energy surface at finite temperatures. Then we will show some results on the phase transition between the B1 and B2 structures in MgO and on the thermodynamic properties of iron.

# TIDAL RESPONSE OF THE ICE-OCEAN SYSTEM ON ENCELADUS

# Hellard, Hugo

Institute of Planetary Research, DLR, Berlin, Germany

The Saturnian moon Enceladus is one of the most geologically active bodies in the solar system with active cryovolcanism restricted to the South Polar Terrain [1]. The rotational state of Enceladus indicates that a global subsurface ocean mechanically decouples the outer ice shell from the satellite's deep interior [2]. We investigate how the interior structure and related dissipation of tidal energy on Enceladus affect the lateral layering of its outer ice shell and the core density. Structural models are created that satisfy the satellite's mean density and polar moment-of-inertia factor as derived from Cassini gravity field data [3]. We particularly consider variations in core density, ice shell thickness and ocean composition. We propose a method to derive lateral variations of the rheological boundary between the brittle and ductile ice layers, based on the assumption that the dissipation of tidal energy is restricted to the ductile sublayer of the outer ice shell. We first calculate the degree-2 body tide Love numbers for our structural models and obtain diurnal tidal stresses at the satellite's surface due to eccentricity tides [4]. Since the total ice shell thickness is small compared to the satellite's mean radius (less than 10%), we apply a thin shell approximation to compute localized tide-induced dissipation and surface heat flow patterns using a Maxwell rheology model [5]. The dissipation of tidal energy induced by the eccentricity tides results in a polar surface heat flow roughly five times higher than the equatorial one. This may have an effect particularly on the polar surface temperature that is governed by the mean daily insolation. The total ice shell thickness is found to decrease with higher core density in order to keep the ocean density within a realistic range for saltwater below 1250 kg m<sup>-3</sup>. A partly hydrated core is compliant with current estimates of ice shell thickness, the amount of tidal heating, and hydrogen abundances in the plumes. The possible existence of a hydrated core implies hydrothermal exchange processes between the latter and the ocean, which would be essential for Enceladus' astrobiological potential. **References:** 

[1] Spencer, J. and Nimmo, F.: Enceladus: an active ice world in the Saturn system, Ann. Rev. Earth Planet. Sci. 41, 693-717, 2013.

[2] Thomas, P. et al.: Enceladus's measured physical libration requires a global subsurface ocean, Icarus 264, 37-47, 2015.

[3] Iess, L., et al.: The gravity field and interior structure of Enceladus, Science 334, 78-80, 2014.

[4] Wahr, J. et al.: Modeling stresses on satellites due to nonsynchronous rotation and orbital eccentricity using gravitational theory, Icarus 200, 188-206, 2009.[5] Beuthe, M.: Tides on Europa: the membrane paradigm, Icarus 248, 109-134, 2015.

# SUPERCRITICAL SILICATE MELTS DURING AND IN THE AFTERMATH OF THE GIANT IMPACT

# Caracas, Razvan

CNRS, École Normale Superieure de Lyon, Laboratoire de Géologie de Lyon, Lyon, France

We employ large-scale molecular dynamics simulations to understand the physical and chemical behaviour of the magma ocean during the Giant Impact and the first stages of crystallization of the resulting magma ocean. We use the densityfunctional theory to compute the forces under which the atoms move according to Newtonian mechanics. For this we employ the VASP implementation. Under pressure we find an increase of the coordination number of all atomic species, as a mechanism for accommodating compression, and a linear decrease of the selfdiffusion. Iron atoms exhibit a gradual reduction of their magnetic moment. The presence of volatile species does not change the compressibility, but considerably affects the diffusion, the melt being less viscous by almost one order of magnitude. At high temperatures we identify the supercritical region characterized by one homogeneous fluid, rich in ionic species. We show that the chemical speciation is very different from the one obtained at ambient pressure conditions. At lower temperatures, in the 2000 – 4000 K, and low density, we capture the nucleation of bubbles. The vapour is formed mainly of isolated ionized small clusters of atoms. When volatiles are present they are the first one populating the bubbles. They enhance the bubble nucleation and favour the gas-liquid separation. They promote incongruent vaporization.

# TOP-DOWN AND BOTTOM-UP FREEZING IN A FE-FES LUNAR CORE

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Since the Apollo era it is well known that the Moon's crust is remanently magnetized [1]. Paleomagnetic studies suggest that a dynamo operated in the Moon's core for a substantial amount of time from at least 4.25 Ga to potentially 1.3 Ga ago [e.g. 2,3,4,5]. One viable mechanism for magnetic field generation is thermo-chemical convection driven by core crystallization [6,7]. The lifetime of the core dynamo is determined by the crystallization scenario, which in turn vitally depends on the relative slopes of the liquidus and the core temperature. If the pressure gradient of the liquidus is greater than the one of the core temperature, freezing will commence at the bottom of the core. In the opposite case, the core starts to freeze at the top. Given that the Moon's core features low pressures, the core might start to crystallize iron at the top for a considerable range of core sulfur concentrations on the iron-rich side of the eutectic [8]. A consequence is the emergence of a snow zone with settling iron crystals on top of a deeper liquid core that convects due to the remelting of those iron crystals [9,10]. In this so-called iron snow regime the lifetime of the thermo-chemical dynamo in the deeper core is determined by the time it takes for the snow zone to grow across the entire core. Those lifetimes can vary depending on several parameters, e.g. the core sulfur concentration, but are generally found to be short and may not be substantially longer than 1 Gyr [10]. Furthermore, it has been suggested that bottom-up core freezing in the Moon's core shifts to top-down crystallization as a consequence of increasing sulfur concentration in the outer core [6]. As soon as this shift has occurred, dynamo activity probably shuts down rapidly since the dynamo region vanishes quickly whenever a snow zone grows. We want to build upon existing thermo-chemical studies and further explore which core crystallization scenario we find for a given core sulfur concentration. Moreover, we investigate the lifetimes of an iron snow dynamo in the Moon's core as well as the timing of the shift from bottom-up to top-down crystallization. To do so, we employ a 1D thermochemical evolution model of the Moon that includes the evolution of the mantle and the core [10,11,12,13]. The liquidus for the ironrich Fe-FeS alloy is taken from [14]. We find that the iron snow regime occurs for a broad range of core sulfur concentrations from 7 wt% to 20 wt%. Bottom-up freezing occurs only for sulfur concentrations less than 7 wt%.

It can be shown that for a lunar core starting to crystallize in the iron snow regime (top down) the resulting dynamo lifetimes are strikingly short (< 19 Myr) and may not explain the oberserved magnetization. Slower core cooling, for instance due to an increased reference mantle viscosity (i.e., assuming stiffer mantle material), cannot prolong the dynamo lifetime. For these cases, only the onset of core freezing is retarded. Alternatively, assuming a low sulfur content, the lunar core can start with bottom-up core freezing that later transitions to top-down freezing. For example, this transition occurs 726 Myr after the onset of inner core freezing if the core has an initial core sulfur concentration of 1 wt%. Those roughly 700 Myr can explain the lifetime of the lunar dynamo up to 3.56 Ga ago and possibly a few hundred million years longer assuming an early thermal dynamo before the start of crystallization. The dynamo lifetime can be doubled to 1.5 Gyr by increasing the viscosity of the mantle from  $10^{19}$  to  $10^{22}$  Pa s. However, this scenario can still not explain the recently extended lifetime of  $\sim 2$  Gyr.

A possibility for slowing down core cooling and thereby extending dynamo activity could be the existence of radioactive heat sources in the core or an Ilmenite layer above the core-mantle boundary.

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# LIGHT ELEMENT DIFFUSION IN LIQUID FE FOR P-T CONDITIONS OF THE EARTH'S INTERIOR

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Chemical diffusion of light elements in liquid Fe plays an important role both during core formation and the growth of the inner core. However, relevant conditions are difficult to achieve in the laboratory, and first-principle determination of the diffusion constants have lacked benchmarking with experiments. Here we present results that combine experimental and computational estimates on diffusivities of Si and O in liquid Fe, covering the whole P-T range from ambient pressure to conditions of the Earth's inner core. We show that both approaches are compatible and use structural information from the molecular dynamics simulations to analyze the experimental results. Si diffuses at a comparable rate to Fe over the whole P-T range considered, which is consistent with the short-range structure in the liquid. For O in Fe, an analysis of the radial distribution function and coordination number reveals that Fe and O compress in a very different manner up to a density of approximately 8 g/cc, with initial compression primarily accommodated by an increase in coordination. This behavior can account for the very anomalous diffusion behavior observed in experiments with no appreciable P-dependence up to 25 GPa.

#### ELECTRICAL RESISTIVITY OF LIQUID IRON WITH HIGH CONCENTRATION OF LIGHT ELEMENT IMPURITIES

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The Earth's outer core mainly consists of liquid iron, enriched with several weight percent of lighter elements, such as silicon, oxygen, sulfur or carbon. Electrical resistivities of alloys of this type determine the stability of the geodynamo. Both computational and experimental results show that resistivites of Fe-based alloys deviate significantly from values of pure Fe. Using optical conductivity values computed with the Kubo-Greenwood formalism for DFT-based molecular dynamics results, we analyze the high-P and T behavior of resitivities for Fe-alloys containing various concentrations of sulfur, oxygen and silicon. As the electron mean free path length in amorphous and liquid material becomes comparable to interatomic distances at high P and T, electron scattering is expected to be dominated by the short-range order, rather than T-dependent vibrational contributions, and we describe such correlations in our results. In analogy to macroscopic porous media, we further show that resistivity of a liquid metal-nonmetal alloy is determined to first order by the resistivity of the metallic matrix and the volume fraction of non-metallic impurities.

# CRYSTAL STRUCTURE OF MGO ALONG THE SHOCK HUGONIOT

# Wicks, June

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Of the more than 6,000 confirmed and candidate extrasolar planets discovered to date those that are 1-4 times the radius of the Earth are found to be the most abundant. The silicate compounds that dominate the EarthâĂŹs mantle likely dissociate into component oxides at the extreme pressures (200-2,000 GPa) and temperatures (5,000-10,000 K) corresponding to conditions of super-Earth mantles. Magnesium oxide (periclase), an end-member of the ferropericlase solid solution (Mg,Fe)O and an important component the Earth's mantle, has been studied under static compression in the pressure and temperature range found within the Earth ( $\sim$  135 GPa, 2500-4000 K). However, as static compression techniques are typically limited to peak pressures of < 200 GPa, much less is known about its behavior under high-pressure and -temperature conditions.

In this study, the structure of MgO upon shock compression over the 200-700 GPa pressure range was examined at the Omega-EP Laser facility at the Laboratory for Laser Energetics, University of Rochester. Laser drives of up to 2 kJ over 10 ns focused onto a polyimide ablator were used to shock compress 50- $\mu$ m thick polycrystalline or single-crystal MgO. At peak compression, the sample was probed with He- $\alpha$  X-rays from a laser-plasma source. Diffracted X-rays were collected using the PXRDiP diagnostic which consists of image plates lining the inner walls of a box attached to the target package. For each pressure we measure crystal structure, pressure (velocity interferometry), density (x-ray diffraction) and shock temperature (pyrometry). Along the shock Hugoniot MgO transforms from B1 to the B2 structure at ~ 400 GPa and melts at ~ 700 GPa. Additional experiments using a decaying shock geometry combined with temperature measurements at the shock front provide a continuous measurement of pressure and temperature changes across the B1-B2 and B2-liquid phase boundaries.

## STABILITY OF THE RHOMBOHEDRAL PHASE IN VANADIUM AND AMBIENT TEMPERATURE COMPRESSION CURVE

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Vanadium metal behavior under high pressure conditions has been the subject of several studies in recent years, both experimental and theoretical. The unexpected body centered cubic to rhombohedral phase transition has been reported first experimentally, followed by several theoretical studies, which predict a second rhombohedral phase and ultimately above 3 megabar pressure the reentry into the stable high pressure bcc phase. Experimental reports so far addressed only the phase transition into the first rhombohedral phase, and have found no evidence of the second rhombohedral phase. In this paper we present our latest experimental results on vanadium compressed in diamond anvil cell to few megabar pressure and will address the stability of the rhombohedral phase of vanadium.

# HYDROCARBONS AT EXTREME CONDITIONS Hartley, Nicholas

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Light elements are the primary constituent of 'icy giant' planets such as Uranus and Neptune within our own solar system, and increasing numbers of extrasolar planets. Due to the forces within such bodies, materials are compressed to many times solid density, with thermal energies on the order of, and even above, the strength of chemical bonds. Under such conditions, significant structural changes occur, such as diamond formation from hydrogen-carbon demixing and novel lattice structures. On experiments at LCLS, plastic samples were shock-compressed to conditions comparable to planetary interiors (150 GPa, 6000 K), with the evolution of the structure was observed by angularly and spectrally resolved X-ray scattering. In the case of polystyrene targets, strong peaks characteristic of a diamond structure was observed. Changes in the amorphous and liquid structures were also measured at different conditions, reached with different drive beams. The results are compared to those from ab initio simulations, with their relevance to planetary evolution and possibilities for future work also explored.

# FAST X-RAY DIFFRACTION OF (MGFE)O ACROSS THE SPIN TRANSITION UNDER DYNAMIC COMPRESSION

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(MgFe)O is the second most abundant mineral in Earth's lower mantle [1]. At pressures corresponding to the lower mantle (between 40 and 60 GPa) Fe2+ changes its electronic configuration from high spin (HS) to low spin (LS) by pairing 3d-electrons [2]. This spin transition affects density as well as compressional and bulk sound velocities (Marquardt et al. 2009) with possible implications for the interpretation of seismic data and dynamic processes in Earth's mantle. Previous experiments to characterize the elasticity of (Mg,Fe)O have been done at either very high frequencies (Brillouin Scattering, Impulsive Light Scattering, Inelastic scattering) or using static x-ray diffraction experiments [3]. Here we present a x-ray diffraction study of (MgFe)O across the spin transition under dynamic compression at room temperature employing different compression rates ranging from 5, 7.5, 9.7 to 18.3 GPa/s to detect a possible compression rate dependence of the spin transition. Dynamic Driven Diamond Anvil Cell (dDAC) experiments have been carried out at the Extreme Conditions Beamline, PETRA III, DESY. Superfast collection of x-ray diffraction images is facilitated through the use of very fast and sensitive detectors. In our experiments, up to 10 diffraction images per second have been collected making it possible to follow the spin crossover as a function of dynamic compression. Since polychromatic (or pink) beam provides more flux than monochromatic beam, diffraction images are more intense and the data collection is faster at the cost of peak broadening and consequently worse resolution. We compare different experiments with monochromatic and pink beams seeking the best conditions for the characterization of (MgFe)O by fast x-ray diffraction. Initial data analysis indicate deviations at pressures above 60 GPa in low-spin (MgFe)O) when comparing our experimental results to EOS provided by previous static-pressure experiments [4]. Data analysis is ongoing to understand the cause of the observed deviations. Bibliography

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# OPTICAL MEASUREMENTS OF THE ELECTRONIC AND TRANSPORT PROPERTIES OF MOLECULAR, OXIDE AND METAL SYSTEMS AT DEEP PLANETARY INTERIOR CONDITIONS

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The transport properties of minerals and fluids at extreme pressure and temperature determine the dynamics of planetary deep interiors, including heat transport, fluid flow, and generation of magnetic fields, as well as phase separation and mixing. Measurements of thermal, optical, electronic, and viscous transport in planetary materials with a combination of static and dynamic high pressure laboratory techniques have recently added significant new constraints on these dynamical systems in both terrestrial and giant planets. Thermal conductivity measurements in metals at high pressure and temperature indicate a low thermal conductivity of Earth and terrestrial planet cores. This suggests a long-lived magnetic field on Earth, as required by paleomagnetic measurements, may be explained without high interior temperatures or unusual core energy sources in the far past. However, the onset of metallic behavior in mantle melts at extreme pressure suggests dynamo processes in rocky mantles may contribute to the magnetic fields of hot terrestrial planets, including the young Earth. Temperature-induced transformations to conducting states are found to be common to all planet-forming insulators under pressure, from elemental sulfur at several hundred K to neon at  $\sim 20,000$  K  $(\sim 2 \text{ eV})$ . These studies have implications for the metallization of hydrogen and helium-neon phase separation in giant planets, with deep sedimentation of noble gases in smaller gas giants potentially explaining the relatively larger core of Saturn compared to Jupiter. New approaches to measuring high pressure viscosity in planetary fluids will also be discussed.

# FORMATION OF METASTABLE PHASES OF SILICON AND GERMANIUM

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Pressure-induced phase transformations in Si and Ge have been much studied using both traditional high-pressure devices such as diamond-anvil cells (DACs) and uniaxial loading via indentation. In this work we have exploited our understanding of the phase-transformation pathways of both Si and Ge gained from indentation to shed new light on the nucleation of metastable phases formed on decompression and heating in a DAC. In situ powder x-ray diffraction was performed at High Pressure Collaborative Access Team (HPCAT), Advanced Photon Source, Argonne National Laboratory. DACs were prepared to either create a quasihydrostatic environment by placing only a small volume of sample in the cell and an higher shear environment by using a larger volume of sample. Neon gas was used as the pressure medium in most cases. Pressure was applied and released using HPCAT's membrane pressure control system with some cells heated in-situ using external resistive heaters. Ex-situ heating of indented Si suggests the formation of a new metastable phase arising from either the rhombohedral r8-Si or the cubic bc8-Si phase. The new phase was named 'Si-XIII' due to a lack of information about its structure. A series of in-situ annealing DAC experiments were conducted to attempt to form Si-XIII in a DAC and measure its structure. However, in the DAC, bc8-Si transformed to the hexagonaldiamond structure at elevated pressure, consistent with previous studies at ambient pressure. In contrast, r8-Si transformed directly to diamond-cubic Si at a temperature of 255°C. These data were used to construct diagrams of the metastability regimes of the polymorphs formed in a DAC however, in contrast to the indentaton-induced regions, no clear formation of Si-XIII was observed. Indentation studies also prompted a DAC study of the compression of Ge. Residual indents made in Ge often contained the r8-Ge phase which had not been widely reported to form after decompression in a DAC. To investigate this, metallic ( $\beta$ -Sn)-Ge was created by loading up to 18 GPa using a membrane system to control the loading and unloading rates. Unexpectedly, in quasihydrostatic conditions, a transition from ( $\beta$ -Sn)-Ge to the rhombohedral r8-Ge phase was always observed independent of the unloading rate. Such quasihydrostatic unloading conditions resulted in the nucleation of the r8 phase, followed by the cubic bc8 and the hexagonal diamond phase. This pathway was also observed after indentation of Ge. In contrast, the non-hydrostatic environment yielded the tetragonal st12 phase. Thus shear is thought to play a major role in determining the phase transformation pathway of Ge.

# JUPITER AND URANUS IN LIGHT OF CURRENT MISSION (PLANNING)

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Among the giant planets in the Solar system, Jupiter currently receives the largest medial attention due to the current Juno mission. NASA' Juno Orbiter, launched in 2011, is designed to accurately measure the gravity field in order to improve our understanding of the winds, the interior, and the formation of Jupiter. Here I will show that the first accurate observational determination of the gravitational harmonics J6 and J8 [1] indicate that the winds are confined to regions well above the hydrogen metallization level at  $\sim 0.5$  Mbar ( $\sim 0.9$  RJup) [2,3], in agreement with predictions based on Ohmic dissipation of the internal magnetic field [4]. Meanwhile, the ice giants Uranus and Neptune have consistently been proposed for a next generation outer Solar system mission. I will explain (i) the importance for an accurate heat flow measurement and (ii) the linked need to investigate the mixing behavior of ices with rocks: despite tremendous uncertainties in internal structure, current Uranus models predict a warm, icy interior mixed with rocks [5].

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# EXPLAINING JUNO'S MAGNETIC FIELD OBSERVATIONS

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Since nearly a year, NASA's Juno spacecraft is orbiting Jupiter. First magnetic field data reveal that the planet's magnetic field is rather patchy with strong smaller scale contributions. We employ numerical dynamo simulations to understand the origin of these interesting features. Jupiter's interior is characterized by a strong density stratification that we model in an anelastic approximations. Our electrical conductivity model profile represents the most important elements: A strong increase with depth in the molecular outer shell and a smooth transition to the conductivity of the metallic hydrogen layer around 87% of the planetary radius. The simulations suggest that the large scale field already known from pre-Juno missions is maintained at depth in the metallic region. Strong low to mid-latitude magnetic patches reminiscent of the Juno observation, however, are produced at the transition region where the fierce zonal winds excited in the outer shell reach down to sizable conductivities. Juno's measurements also show a weaker or even invers field north of 60 deg. latitude. This is a typical feature observed inside the tangent cylinder of many geodynamo simulations but not in our Jupiter mode that assumes a smaller inner core. (The tangent cylinder is an imaginary boundary that touches the inner core equator.) The observation thus suggests that Jupiter's rocky core may occupy up to 50% of the planetary radius.

# ELECTRICAL AND THERMAL CONDUCTIVITY OF PARTIALLY IONIZED WATER PLASMAS

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The equation of state and transport properties of warm dense water are of fundamental importance for understanding the interior structure and magnetic-field generation in water-rich giant planets like Uranus and Neptune. Standard adiabatic structure models for these planets use mainly thermodynamic properties as input (see Refs. [1,2] for thermodynamic potentials for the dense water ices VII and X and for superionic water). In addition, the thermal conductivity of planetary matter becomes a key quantity when determining whether or not stably stratified or semi-convective layers exist inside a planet. Such regions result in non-adiabatic interior profiles and may offer a possible explanation for Uranus' unusually low luminosity [3]. Here we employ a combination of density functional theory (DFT) and molecular dynamics (MD) simulations to calculate the electrical and thermal conductivity of water plasmas. We focus on the electronic contribution to the conductivities, which we determine using expressions from linear response theory [4]. We investigate both expanded and compressed states of water between densities of 0.1 and 10 g/cm<sup>3</sup> and temperatures up to 50 000 K and parametrize our data with analytic functions. Furthermore, we also give an estimation for the nuclear contribution to the thermal conductivity in dense water plasmas based on our DFT-MD simulation data. Depending on the density and temperature conditions, the nuclear contribution may be of comparable or even larger importance than that of the electrons. Our results contribute to understanding conduction processes in complex multicomponent plasmas and are relevant for the physics of planetary interiors as well as for technical plasma applications. This work is supported by the Deutsche Forschungsgemeinschaft (DFG) within SFB 652, SPP 1488, and FOR 2440.

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# THERMAL AND OPTICAL PROPERTIES OF DENSE HELIUM Preising, Martin

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We studied the behavior of solid and fluid helium under high pressure with molecular dynamics simulations based on density functional theory (DFT-MD). Helium, as the second abundant element in nature, is important for astrophysical applications, e.g., the interior and evolution of gas giants and brown dwarfs. In particular, we calculated the melting line and examine the insulator-to-metal transition, both for 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 [Robert et al., Phys. Rev. E 91, 033310 (2015)]. We have implemented this method and investigated finite-size effects and other convergence issues. We found good consistency with available experiments and gave predictions for the melting line of helium up to the TPa region. Laser-driven compression experiments have shown that helium undergoes an insulatorto- metal transition with increasing density and temperature [Celliers et al., Phys. Rev. Lett. 104, 184503 (2010)]. However, the exact location and nature of this transition is not clear yet. From the temperature and reflectivity measurements, the DC conductivity was inferred using a simple Drude model. We performed extensive DFTMD simulations for the reported conditions and calculated the reflectivity and DC conductivity employing the Kubo-Greenwood formalism [Holst et al., Phys. Rev. B 83, 235120 (2011)] and the PBE, vdW-DF1, and HSE exchangecorrelation (XC) functionals. We found a significant impact of the XC functional on the DC conductivity, especially at lower densities and temperatures. We compared our results with available data [Celliers et al., Phys. Rev. Lett. 104, 184503 (2010), Soubiran et al., Phys. Rev. B 86, 115102 (2012)].

# INSIGHTS INTO THE EARTH'S CORE THROUGH GEOMAGNETIC DATA ASSIMILATION

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The geomagnetic field is generated by a natural dynamo mechanism taking place in the Earth's outer core. Direct and indirect observations of the field at the surface and in altitude can provide means of estimating the geomagnetic field at the core mantle boundary and at some extent the flow immediately underneath. However, a more complete understanding of the whole core dynamics can be sought by combining observations and numerical models of the dynamo, through data assimilation. Data assimilation is a framework consisting of different time-dependent inverse methods, where the main goal is to use all available information to estimate the state of a physical system. In this talk, we will see how such methods can be applied in geomagnetism - to either analyze past and present configurations of the hidden part of the dynamo, like the flow and magnetic fields inside the core, to forecast the evolution of the observed magnetic field, and to estimate the initial conditions and control parameters governing the system.

# THERMAL EVOLUTION AND CORE STRATIFICATION OF MERCURY

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Like the Earth, Mercury has a global magnetic field that is powered by convective motions in its liquid iron-rich core. Convective motions are mainly generated by iron-alloy crystallization, light element exsolution, and secular cooling. Thermal evolution studies indicate that the present-day heat flow at the core mantle bound-ary of Mercury is subadiabatic. As a consequence a stable thermal boundary layer could form at the top of its core. Additionally, the formation of iron-rich snow and chemical reactions between the mantle and the core could lead to the formation of a chemically stable layer in the core. A stable upper core thermally conductive layer reduces the core cooling rate, affects the inner core evolution, and the dynamo action. In this study, we use a coupled thermal evolution model of the core and mantle to constrain the interior structure of Mercury. We assess conditions for the formation of a stable stratified layer in the core and study how it affects the evolution of the inner core and core dynamo action.

# RESOLVING DYNAMIC PROPERTIES OF WARM DENSE MATTER

# Rohatsch, Katja

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Warm dense matter (WDM) is an extreme material state which can be found in the interior of stars, large planets and brown dwarfs but also in laboratory experiments, where solid matter is quickly transferred to a plasma state. Densities in the region of solids and temperatures in the region of  $10^4 - 10^5$  K represents the prevalent thermodynamic conditions. Complex dynamic processes, partial ionization, electron degeneracy and ion-coupling makes the characterization of WDM very challenging and requires the development of new theoretical models. X-ray free electron lasers in combination with high-energy high-intensity optical lasers provide unique possibilities to create and probe WDM states and their dynamic properties in the laboratory. Due to the enormous temporal resolution the dynamics of processes like e.g. non-thermal melting or coulomb crystallization can be studied, which offer required tests of model predictions. This poster will present an experiment performed at the MEC instrument at LCLS which investigated ultrafast melting in SiO2. It also will show planned experiments with HIBEF at the HED user facility at European X-FEL, focusing on the study of dynamic properties of WDM.

# STRUCTURAL AND THERMAL MODELS OF ROCKY PLANETS AND SOLID EXOPLANETS Sohl, Frank

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This subproject aims at improved relationships between mass, radius, bulk composition, and the thermal state of transiting exoplanets based on novel material laws obtained within the Research Unit and addresses the following key questions: -What is the interior structure and thermal history of rocky planets? - How can we distinguish between super-Earths and mini-Neptunes? Since the convective energy transport in the silicate mantles of massive super-Earths could be inefficient owing to pressure effects on viscosity, the interplay between internal heat production, secular cooling and intrinsic luminosity or surface heat flow will be studied in detail. Furthermore, the robustness of mass-radius relationships and their usage for the classification of low-mass solid planets up to ten Earth masses will be investigated. Moreover, the determination of key tidal parameters such as the fluid Love number  $k_2$ , f will allow to infer the tri-axial global shape of tidally locked close-in planets for additional comparison with astronomical lightcurve variations.

# A STABLY STRATIFIED LAYER IN SATURN'S INTERIOR Dietrich, Wieland

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The thermal evolution of Saturn, its magnetic field morphology, as well as implications from ring seismology and the high-pressure, high-temperature demixing behaviour of H/He support the concept of a (compositional) stable stratified zone suppressing convective heat transport for roughly 15% of the planetary radius. This stable stratified layer (SSL) is then sandwiched between a deep-seated convective dynamo region, where the electrical conductivity due to metallic hydrogen is sufficient, and a non-magnetic outermost convective zone generating the fierce geostrophic zonal winds observed at the surface. Even though convective instabilities are strongly suppressed in the SSL, it might be enriched with gravity waves and thermal wind driven zonal flows. For decades, is has been (and still is) rather challenging to reproduce Saturn's characteristic magnetic field and zonal wind pattern in global 3D MHD models, e.g. by using this probably quite essential stable layer. However, our new numerical model aims to more realistically capture Saturn's internal properties and interior dynamics by modelling a mid-depth SSL as a deviation from the adiabat and, additionally, using a radial profile of electrical conductivity. For this talk, we will present the physical and numerical setup for a model of Saturn's global atmospheric dynamics as well as show first results from hydrodynamic simulations. Our method is capable of generating a stable layer comparable to the one in Saturn, e.g. in terms of the Brunt-Väisälä-frequency. We report choice and dependence of the key parameters to keep the physics meaningful and the numerics feasible at the same time. In particular, the generation of geostrophic and ageostrophic zonal flows driven by the interplay of convection, thermal winds and a stable (non-convecting) region is discussed.

# TOWARDS A NEW TOOL FOR MODELLING GIANT PLANETS

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We present work in progress towards a modelling approach for the interior and evolution of giant planets. It follows the well-known method by Henyey et al. (1964) [1] for stars. The equations of mass conservation, hydrostatic equilibrium, energy balance and transport are solved for each time step iteratively and then passage of time is applied via the energy balance equation. In contrast to conventional modelling assumptions for Jupiter and Saturn [2] and Uranus and Neptune [3], our goal is to go beyond the premise of adiabatic interiors, as the presence of stably stratified and thus non-adiabatic regions is indicated by some magnetic field models for the ice giants [4]. Therefore, we solve selfconsistently for the local temperature gradient, the compositional gradient and the heat flux, accounting for heat and particle transport by convection and diffusion. Thus, we hope to gain new insight into the origin of the low intrinsic luminosity of Uranus and high intrinsic luminosity of Neptune. To this end, a new computer code is developed. Here, we present the theoretical groundwork of our model as well as preliminary test results.

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# ESTIMATING THE DEPTH OF THE DYNAMO IN JUPITER

# Duarte, Lucia

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Jupiter's magnetic field is currently being observed by the Juno spacecraft in more detail than ever before. Since its interior is likely fully convecting, Jupiter's observations provide a good insight into the interior dynamics that sustain the dynamo. The interior of Jupiter is divided in three layers: a rocky inner core and two outer layers mainly composed of hydrogen: molecular and weakly conducting closer to the surface and metallic and electrically conducting in the deep interior. Since there is still a lot of uncertainty on the actual interior dynamics, we do not know where dynamo action starts.

From pre-Juno measurements, we only had access to the largest scales where the dipole component of the field dominates. Juno will be able to access a lot of the information "hidden" in the smaller scales. By constraining better the slope of the power spectrum for example, we may also infer about the depth of the dynamo through a potential field extrapolation. In this work, we take a set of Jupiter-like simulations selected based on comparison with pre-Juno data and we analyze in more detail the interior dynamics of these models. Based on the ab initio radial profile of electrical conductivity for Jupiter, we vary this gradient to explore the changes in the dynamics. Finally we explore a few different ways to estimate the top of the dynamo region from the surface spectrum, that could eventually predict this upper boundary with some certainty independently of the complex interior dynamics.

# MODELLING YOUNG HOT JUPITERS AS A WINDOW TO FORMATION PROCESSES

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We aim at understanding giant planet formation processes and evolution scenarios of planetary systems. Basic correlations such as that between the planetary heavy element mass (MZ) and the stellar metallicity [1] are key in this context. We determine the planetary heavy element mass by thermal evolution and structural models. Structural models require an atmosphere model as an outer boundary condition. The atmosphere model describes the coupling between the convective interior, where pressures reach up to several 10 Mbar, and the stellar radiation field. In particular, the radiation transport through the atmosphere influences the cooling of the planet during the evolution and thus the present interior structure. Here we investigate the influence of different atmosphere models [2,3] on the derived heavy element mass of young single planets such as the 300 Myr old Hot Jupiter WASP10b. We find that the uncertainties in the atmospheric temperature may lead to an uncertainty in MZ of up to 100 ME. In future work, we will compare to the uncertainty due to the applied high-pressure H/He EOS, which in case of brown dwarfs was found to be a factor of two [4].

References:

[1] Guillot et al. 2006, A 453:L21

[2] Fortney et al. 2007, ApJ 659:1661

[3] Guillot 2010, A 520:A27

[4] Becker et al. 2014, ApJS 215:21

# REFINING EMPIRICAL CONSTRAINTS ON THE TRANSPORT PROPERTIES OF EARTH'S CORE

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