# Classical Charged Systems Session 1

## Dusty Plasmas: Model Systems to Investigate Coupling Dynamics and Anisotropic Effects

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The stability of structures and transport of energy are affected by the coupling between elements in the system. A dusty plasma is an ideal system to investigate coupling effects as the individual dust grains can be easily imaged and the coupling can be tuned by changing the plasma parameters. The key to understanding the coupling strength is determining the dust charge and the shielding provided by the plasma environment. The simplest theory of dust charging assumes that dust grains are isolated spheres in an isotropic, homogeneous plasma. However, experimental and theoretical studies reveal that the charge collected by a dust grain depends on many factors such as the shape and material of the grain, plasma flow, and the presence of magnetic fields. Anisotropic plasma shielding arises from ion wake structures formed downstream of the dust grains in a flowing plasma, creating directional variations in energy transport and coupling. These ion wakes can be incorporated into kinetic models as an effective dust potential. This talk will give an overview of dust charging in non-homogeneous plasmas. Variation in the effective dust potential, driven by anisotropic shielding, leads to diverse dynamical effects such as anomalous diffusion, unique wave modes, distinct phase transitions, mode-coupling instabilities, visco-elastic dissipation, liquid crystalline dust structures, and active matter systems.

Support for this work from the US Department of Energy, Office of Science, Office of Fusion Energy Sciences under awards DE-SC0024681, the National Science Foundation under award numbers PHY-2308742 and PHY-2308743, NSF EPSCoR FTPP OIA-2148653 is gratefully acknowledged. All authors acknowledge the joint ESA/Roscosmos Experiment Plasmakristall-4 (PK-4) onboard the International Space Station.

## Bulk viscosity of strongly coupled plasmas

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Bulk viscosity of the one-component plasma (OCP), a model system for strongly coupled atomic plasmas, is computed using molecular dynamics simulations [J. LeVan and S.D. Baalrud, Phys. Rev. E 111, 015202 (2025)]. Using the Green-Kubo formula, it is found that the bulk viscosity in the OCP is smaller than the shear viscosity for all values of the Coulomb coupling parameter Γ. We also compute bulk viscosity of the rigid rotor one- component plasma (ROCP), a model system for strongly coupled diatomic plasmas [J. LeVan, M.D. Acciarri, and S.D. Baalrud, Phys.

Rev. E 110, 015208 (2024)]. We find that the coefficient of bulk viscosity can exceed the shear viscosity by several orders of magnitude at certain values for Γ and the bond length parameter Ω. This occurs due to the very long rotational relaxation time associated with molecular ions. Although bulk viscosity is often neglected in plasma modeling, our results suggest that plasmas with a large quantity of molecular ions may have a very large bulk to shear ratio. Including bulk viscosity in fluid simulations may enable more accurate modeling of turbulence, shock waves, and instabilities.

This research was supported by the US Department of Energy under Award No. DE-SC0022201.

# Theory of Electron-Ion Temperature Relaxation in Strongly Magnetized Antimatter Plasmas

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Strongly magnetized plasmas characterized by gyrofrequency larger than the plasma frequency are known to exhibit novel transport properties. Here, we study the electron-ion equilibration in strongly magnetized plasmas, specifically focusing on the collisional cooling of antiprotons by electrons within the ALPHA trap for antihydrogen synthesis. We observe that strong magnetization significantly restricts energy exchange between parallel and perpendicular directions during intraspecies collisions (ion-ion or electron-electron), resulting in extended temperature anisotropy relaxation times. Consequently, during ion-electron equilibration, neither species maintains an isotropic Maxwellian distribution. The anisotropy evolution becomes a critical factor in determining the temperature evolution of ions and electrons during equilibration. We derive a general evolution equation for the temperatures and anisotropies of both ions and electrons. It is found that when electrons are strongly magnetized, and ions are weakly magnetized, the magnetic field significantly suppresses the electron perpendicular energy exchange rate while slightly enhancing the parallel exchange rate compared to the weak magnetization regime. Conversely, both ion perpendicular and parallel energy exchange rates increase relative to their weakly magnetized counterparts. This leads to a rapid alignment of the electron parallel temperature with the ion temperature, while the electron perpendicular temperature equilibrates much more slowly [L. Jose, J. C. Welch, T. D. Tharp, and S. D. Baalrud, Phys. Rev. E 111, 035201 (2025)]. The anisotropy relaxation rates obtained from the theory are in good agreement with the results from the strongly coupled non-neutral plasma experiments [F. Anderegg, D. H. E. Dubin, M. Affolter, and C. F. Driscoll, Physics of Plasmas 24, 092118 (2017)] and the molecular dynamics simulations.

Acknowledgement
This material is based upon work supported by NSF grant awards No.PHY-2205506 and PHY-2205620.

## Bremsstrahlung Emission in Strongly Coupled Plasmas

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Bremsstrahlung emission influences radiation transport in astrophysical, fusion, and industrial plasmas. The warm dense plasmas created in these systems can often be in an intermediate coupling regime, where the average kinetic energy of particles is on the order of the potential energy at the average interparticle spacing. Here, we present mean force emission theory, which attempts to extend the classical theory of bremsstrahlung emission into the strongly coupled regime. Strong coupling effects are observed to cause the emission spectrum to become peaked near the electron plasma frequency. For frequencies above the plasma frequency, we show that the radiation spectrum can be described by solving for the electron trajectory during a binary collision, but where the electron-ion interactions occur through the potential of mean force. Below the plasma frequency, we show that the spectrum can be described using an autocorrelation formalism that captures the effect of multiple collisions in sequence. Predictions of the model are benchmarked using classical molecular dynamics (MD) simulations of a repulsively interacting two-component plasma. The theory is also applied to attractively interacting systems by using a pseudopotential to model the electron-ion interaction. In the high frequency limit, the pseudopotential leads to a decay of the emission coefficient in a qualitatively similar way as the repulsive case. The pseudopotential also allows for classically bound states to form in the MD simulations, and this leads to peak in the emission spectrum that is absent in the repulsive case. [J. P. Kinney, H. J. LeFevre, C. C. Kuranz, S. D. Baalrud; Mean force emission theory for classical bremsstrahlung in strongly coupled plasmas. *Phys. Plasmas* 1 May 2024; 31 (5): 053302].

This work is funded by the NNSA Stockpile Stewardship Academic Alliances under grant number DE-NA0004100 and the DOE NNSA Stockpile Stewardship Graduate Fellowship through cooperative agreement DE-NA0003960.

# High-Energy Density Plasmas in the Laboratory Session 1

## First fusion laboratory experiments to achieve target energy gain >1

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The inertial fusion community has been working towards achieving ignition using high powered lasers for decades, since the idea of laser-inertial confinement fusion (ICF) was first proposed by Nuckolls, et al., in 1972. On August 8, 2021 and Dec 5$^{th}$ 2022, the Lawson criterion for ignition was

met and more fusion energy was created than laser energy incident on the target at the National Ignition Facility (NIF) in Northern California. The first experiment produced a fusion yield of 1.35 MJ from 1.9 MJ of laser energy and appears to have crossed the tipping-point of thermodynamic instability according to several ignition metrics [1-3]. Building on this result, improvements were made to increase the fusion energy output to ~4MJ from 2.05 MJ of laser energy on target [4-6], resulting in target gain exceeding unity for the first time in the laboratory. Since then, we have further increased fusion target gain to ~2.4 times and 5.2 MJ using 2.2 MJ of laser energy. In addition, application of a continuously varying W dopant in the diamond capsule holding the DT fuel, further improved performance by another >2x leading to record target gains of >4. We continue to explore new methods for increased compression and coupling to further improve DT fuel burn up fraction. These results show that there is nothing fundamentally limiting controlled fusion energy gain in the laboratory.

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# Density Functional Theory-Molecular Dynamics (DFT-MD) Simulations for Hydrogen and Mixtures

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Understanding the behavior of hydrogen, helium, oxygen, and their mixtures under extreme pressure and temperature conditions, such as those found in giant planets, remains a significant scientific challenge. While the properties of these elements are well understood under Earth-like conditions, their behavior in high-pressure environments are less explored [Helled2020]. This talk will address key aspects of this frontier.

For pure hydrogen, the focus is on uncovering the details of the first-order liquid-liquid phase transition, which is coupled with the nonmetal-to-metal transition. We use DFT-MD simulations to study these phenomena, investigating the effects of different exchange-correlation functionals. A comparison of our results with experimental campaigns and quantum Monte Carlo simulations shows that the Heyd-Scuseria-Ernzerhof (HSE) functional offers the best agreement [Bergermann2024a].

We also explore the miscibility gaps in H-He and H-$H_2O$ mixtures using DFT-MD simulations[Bergermann2021]. By applying the coupling constant integration method, we

calculate the ionic non-ideal entropy, offering new insights into the interactions of hydrogen, helium, and water under extreme conditions. This comprehensive investigation deepens our understanding of their miscibility gaps and their behavior in planetary interiors [Bergermann2024b].

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# Experimental validation of electron correlation models in warm dense matter

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The plasmon dispersion in warm dense matter (WDM) reveals the details of collective electron behaviour. This study employed advancements in eV-resolution X-ray scattering (XRS) developed at HED-HIBEF at the European XFEL, using seeded X-rays at 8.31 keV to achieve high spectral resolution. These parameters enabled precise measurements of plasmon dispersion in dynamically compressed aluminum. This prototypical metal was chosen for its ease of handling, modelling, compression and diagnostic reliability, as well as the abundance of previous experimental data and simulations. The DiPOLE laser created pressures of 25-50 GPa with extraordinary shot-to-shot stability (1-2%), ensuring highly reproducible results.

Measurements were obtained with a forward scatteing spectrometer at four distinct scattering angles, along with X-ray diffraction (XRD) to track structural changes. The XRD pattern observed in the experiment closely matched the results of simulations combining density functional theory molecular dynamics (DFT-MD) and the HELIOS radiation-hydrodynamics simulations. This agreement enabled accurate determination of density and temperature composition, as well as modeling of the static structure factor S(k).

The dynamic structure factor (S(k, ω)) derived from simulations was compared directly with the measured plasmon data for both ambient and driven conditions, using several state-of-the-art time-dependent DFT models, as well as simpler models based on homogeneous electron gas appoaches. The tight error bars in our measurments allow to observe deviations to certain models. This work represents one of the most accurate measurements of plasmon dispersion under compression, offering a valuable reference for future studies of warm dense matter.

We present this talk on behalf of the entire team of the community proposal EuXFEL #6656 (Kraus/Preston) as co-authors of this presentation.

# Developments in Theoretical Methods and Numerical Techniques Session 1

## Ab initio path integral Monte Carlo simulation of warm dense matter

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Understanding matter at extreme densities, temperatures and pressures is important for the modeling of astrophysical objects (e.g. giant planet interiors) and technological applications (most notably inertial confinement fusion) alike. Yet, the intricate interplay of effects such as Coulomb coupling, quantum degeneracy, and strong thermal excitations renders the rigorous theoretical description of such warm dense matter (WDM) challenging.

Here, I present an overview of a number of recent developments in the ab initio path integral Monte Carlo (PIMC) simulation of WDM [1,2,3]. While being computationally demanding, PIMC is exact within the given error bars and, thus, constitutes a valuable benchmark for computationally more efficient methods such as density functional theory (DFT). Moreover, these simulations open up new avenues for the interpretation of X-ray Thomson scattering (XRTS) measurements, which is a key method of diagnostics for experiments with extreme states of matter. As a practical example, we consider a recent XRTS experiment on strongly compressed beryllium carried out at the National Ignition Facility (NIF) in Livermore [4], for which we find a significantly lower density based on both ab initio PIMC and DFT simulations [3,5] compared to previously used chemical models and radiation hydrodynamics calculations [4].

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## Quantum Monte Carlo data for Neural Network potentials of dense hydrogen

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Dense hydrogen is important for understanding planetary interiors such Jupiter and Saturn but experiment measurements are very limited. Density functional theory gives reasonable results but its accuracy is uncertain and often inadequate. Quantum Monte Carlo (QMC) is very accurate for low Z elements, particularly hydrogen, since one does not need a pseudo potential, effects of antisymmetry are much better controlled and accurate methods are available for determining forces. However, both DFT and QMC are too costly to determine details of the hydrogen phase diagram.

We used machine learning to train a model using hydrogen forces and energies determined by Diffusion QMC on configurations of dense solid and liquid, molecular and atomic hydrogen. We then performed classical and quantum simulations to determine stable phases of hydrogen for pressures in the range of 100-300GPa and temperatures in the range of 200K to 2000K. The resulting phase diagram differs significantly from previous estimates.

Refs.: H. Niu et al., Phys. Rev. Letts. **130**, 076102 (2023), S. Goswami, et al. J. Chem. Phys. **162**, 054118 (2025).

## Study of early-stage carbon plasma formation from laser-irradiated graphene and diamond via ab initio calculations and kinetic plasma simulations

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Irradiating carbon targets with an intense short-pulse laser induces extreme conditions in the material and produces plasma. Understanding the physics of carbon plasma formation is essential for Inertial Confinement Fusion concepts and extensive aspects of astrophysics. However, the details of early-stage plasma formation and dynamics still need to be clarified since experimental investigation of such fast evolution (~fs) is very challenging. Here, we are developing a novel method to investigate this process. First, ab initio electronic structure calculations using the density functional theory molecular dynamic code CHIVES were performed. By varying the initial electronic temperature ($T_e$) and ionic temperature ($T_i$) in the system, critical parameters such as electron density, electron and ion energy, etc., are calculated with a temporal resolution of less than 1 fs. The electronic density of states is analyzed so that the evolution from solid to plasma can be monitored and the critical time of transition can be identified. Given that simulations with realistic experimental size and time are computationally costly, ab initio results are then used as input for further kinetic calculations with a particle-in-cell code WarpX to model the interaction between a short-pulse laser in the order of $10^{14}$ W/cm$^2$ and carbon targets (graphene and diamond). Preliminary results and the comparison between different methods will be discussed. This work provides a first-principles point of view on early-stage plasma formation, and it can be used to identify the impact of atomic configuration on laser-carbon interaction.

This research was supported by funds from the UC Multi-Campus Research Programs and Initiatives of the University of California, Grant Number M23PR5854.

# Nonlinear and linear density response of finite temperature quantum systems

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Density response theory is ubiquitous throughout physics and naturally plays a central role in the theoretical description of warm dense matter. In the ground state, linear density response theory has been exhaustively studied, but there is still ample room for advances in finite temperature systems and concerning non-linear extensions.

In the realm of linear density response theory: (i) We present a formally exact Matsubara-Fourier representation of imaginary time correlation functions (ITCFs) that comprises the imaginary-time generalization of the Matsubara series for equal-time correlation functions. We discuss its utility in the extraction of physics information from path integral Monte Carlo (PIMC) data. (ii) We present a formally exact series that connects any even $2k$ frequency moment of the dynamic structure factor (DSF) with the infinite sum of all odd frequency moments of the DSF starting from the $2k-1$ frequency moment. We discuss its application in the estimate of unknown frequency moments of the DSF. (iii) We present a formally exact expression for the long-wavelength limit of the ITCF that is valid for any imaginary-time. We also present its validation with PIMC data.

In the realm of nonlinear density response theory: (i) We present a formally exact expansion in the non-interacting limit that expresses diagonal arbitrary order nonlinear responses as the weighted sum of the Lindhard responses evaluated at all multiple harmonics. We also discuss its validation with PIMC simulations. (ii) We discuss fundamental problems in the evaluation of non-interacting off-diagonal responses of arbitrary order, which are seemingly divergent.

In the realm of linear density response theory of multi-component systems: (i) We present quasi-exact PIMC data for the spin-resolved density responses and local field corrections of the finite temperature uniform electron gas. (ii) We present quasi-exact PIMC data for the species-resolved density responses and local field factors of warm dense hydrogen.

# High-Energy Density Plasmas in the Laboratory Session 2

## Probing thermodynamic and transport properties of expanded warm dense matter by isochoric heating

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In high-energy-density physics, Warm Dense Matter (WDM) physics has been identified as a challenging research area due to its unique location in the density-temperature map at the junction of plasma, solid and liquid states. Many of the assumptions and approximations that have been successfully applied either in plasma physics or in condensed matter theory do not apply, making it difficult to develop a consistent model for WDM. Over the past decades, exploring this regime has become crucial for laboratory astrophysics or Inertial Confinement Fusion.

For these reasons, a pulsed-power facility has been recently developed at CEA DAM Île-de-France for studying the expanded part of WDM regime. It is based on the pulsed Joule heating technique, originally proposed by Korobenko et al. [1], for inducing a solid to plasma phase transition to metallic foils confined into a sapphire cell [2]. In this presentation, we report about recent experiments conducted on aluminum and copper to assess electrical conductivity and thermodynamic properties across a density range from solid-state values down to 1/8 of the initial density, with pressure reaching up to 12 GPa and temperature ranging from 1 to 7 eV. Experimental results are compared to DFT-MD simulations and various equation of state and conductivity models extracted from the literature. As a result, our experimental data appear to be able to improve significantly the modelling of EOS and electrical conductivity in expanded WDM regime.

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## Characterizing Polymer Foams with Simultaneous X-ray Fluorescence Spectroscopy and Thomson Scattering

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Understanding the behavior of polymer foams at high energy density conditions is crucial to advance inertial fusion energy research. Here, we present data measuring the thermodynamic state of these materials at megabar pressures. At the Matter in Extreme Conditions Endstation of the Linac Coherent Light Source, we heat samples using an optical, high-intensity, femtosecond laser and dynamically probe them with ultra-short, coherent X-ray pulses of high peak brightness. Our data resolve the ultrafast response to laser heating with sub-ps resolution, measuring plasma temperatures exceeding 50 eV. At the OMEGA laser facility, we study spherically converging implosions of foam shells. In both experiments, we perform X-ray Thomson scattering measurements in forward and backward scattering geometries to capture both collective and non-collective electron behavior in the sample. Simultaneously, X-ray fluorescence spectroscopy is used to measure the emission from a mid-Z dopant, providing complementary information on the plasma conditions. By combining these techniques, we obtain temporally resolved temperature measurements of the transient warm dense matter states and lay the foundation for precision studies of wetted polymer foams. These diagnostics are now being fielded on upcoming experiments at EuXFEL and SACLA to investigate foam response under varied drive conditions and further improve data fidelity.

## Linear response time-dependent density functional theory for modeling plasma X-ray Thomson scattering spectra

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In X-ray Thomson scattering (XRTS) experiments, the dynamic structure factor (DSF) of electrons convolved with a probing X-ray beam and the instrument function is measured, allowing for plasma diagnostics under extreme conditions of high energy density and short time scales. Linear response time-dependent density functional theory (LR-TDDFT) is a crucial ab initio method used

to simulate the DSF [1]. In this work, we explore the application of LR-TDDFT for modeling XRTS, with a particular focus on describing experimental measurements and predicting new features arising from the heating and/or compression of solids [2-5], e.g. a thermally induced red shift of the collective plasmon excitation in Al and Si [3] and the thermal changes in the d-band excitations and effective charge of Cu [4] (see the figure). We also consider an alternative approach that employs the Liouville-Lanczos technique for simulating the DSF [5, 6]. This method does not require empty states, enabling us to access the DSF at high momentum transfer values and across a wide range of frequencies. Furthermore, we utilize exact path integral Monte Carlo results for the imaginary-time density-density correlation function to benchmark the Liouville-Lanczos approch to LR-TDDFT [5]. The successful validation of the Liouville-Lanczos method is a significant contribution to the ab initio simulation landscape, supporting experimental efforts in the field of warm dense matter.

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# Experimental Characterization of HED Hydrodynamic Instabilities at Omega EP

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High-energy-density (HED) systems, such as inertial confinement fusion (ICF), are susceptible to hydrodynamic instabilities that can significantly affect both experimental results and modeling predictions. These instabilities can induce mixing across material interfaces, which is a primary contributor to degrading ICF performance. Particularly, instability-driven jetting from interacting defects can be particularly destructive at interior layers. Determining the range of conditions where this occurs as well as our ability to mitigate this effect both require extensive experimental benchmarking of expensive 3D simulations. This talk will detail an experimental platform fielded by Los Alamos National Laboratory at the Omega EP Laser to characterize the effect of defect-driven jetting in HED systems as a part of a larger multi-facility, multi-scale investigative effort.

# Confined and Mesoscopic Coulomb Systems Session 1

## The quantum wonders of 2D Coulomb systems

Shiwei Zhang[1]

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Recent experimental advances, for example, with layered materials and semiconductor interfaces, have provided a plethora of opportunities to study interacting Coulomb systems confined to two dimensions, with exquisite control and precision. The two-dimensional electron gas (2DEG) is a fundamental model in condensed matter physics which can provide key insight to these systems. The model describes interacting electrons in a uniform compensating charge background. Despite its simplicity, determining the ground-state phases of 2DEG has been challenging. The model becomes even more challenging, and much richer, when external potentials are included to model the experiments, for example a periodic moire potential or defects/disorder. Using quantum Monte Carlo methods and new machine learning tools involving neural quantum states, we investigate the 2DEG with and without external potential. I will introduce some of the advances in our capabilities for accurate computations, and then present a number of results which have provided new insights and predictions and promise great synergy with experiments.

## Excitonic superfluidity in electron-hole bilayer systems

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There is accumulating evidence for the existence of quantum condensation of excitons in double layer semiconductor heterostructure devices, with the electrons and holes spatially separated in adjacent parallel conducting layers. This has sparked a lot of interest in excitonic superfluidity at equilibrium. The electron-hole pairing attraction is strong, promising high transition temperatures. Because the attraction is long-ranged, screening controls many superfluid properties. The systems offer the exciting prospect of a tunable electronic device that can sweep across the superfluid BCS-BEC crossover regimes. Pros and cons of different candidate heterostructures are discussed, accompanied by a brief overview of the current experimental status.

## Superfluidity in exciton bilayer systems: collective modes as definitive identification-marker

Filippo Pascucci[1], Sara Conti[1], David Neilson[1], Andrea Perali[2], Jacques Tempere[1]

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Recent discoveries of new bidimensional materials have renewed the attention of researchers about the superfluidity of indirect excitons in systems comprising a conductive layer of electrons close to a conductive layer of holes. Despite extensive experimental efforts, conclusive evidence of exciton superfluidity remains elusive due to challenges in traditional probing methods, partly because of the neutral nature of excitons.

We investigate the behaviour of density collective modes in the normal and superfluid phases of the bilayer exciton system to identify alternative fingerprints of exciton superfluidity. We derive the dressed density response functions through the Random-Phase-Approximation considering a self-consistent screened interlayer and intralayer interaction.

In the normal state, stable acoustic and optic density collective modes exist outside the particle-antiparticle continuum.

In the exciton superfluid phase, screening effects lead to an energy gap in the single-particle excitation spectrum that is consistently larger than the Fermi energy.

We show that such a large energy gap suppresses the propagation of stable density collective modes as the system transitions from the normal to the superfluid exciton phase.

Experimental observation of the disappearance of the acoustic and optic branches would serve as an unambiguous fingerprint of exciton superfluidity in bilayer systems.

# Collective depinning and sliding of a quantum Wigner crystal in two-dimensional electron systems

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I will report the observation of two-threshold voltage-current characteristics accompanied by a peak of broadband noise between the two threshold voltages, $V_{th1}$ and $V_{th2}$, in the insulating state at low electron densities in two-dimensional electron systems in silicon metal-oxide-semiconductor field-effect transistors [1] and ultrahigh mobility SiGe/Si/SiGe heterostructures [2]. As the applied voltage increases, the current remains near zero up to a threshold voltage $V_{th1}$. After reaching $V_{th1}$, the current increases sharply until a second threshold voltage $V_{th2}$ is reached. Beyond $V_{th2}$, the slope of the *V*-*I* curve significantly decreases, and the behavior becomes linear, although it is not ohmic (see Fig. 1). The two-threshold $V-I$ characteristics reported in this paper are strikingly similar to the two-threshold $I-V$ characteristics known for the collective depinning of the vortex lattice in type-II superconductors [3], with voltage and current axes interchanged. The observed results can be described by a phenomenological theory of the collective depinning of elastic structures, which naturally generates a peak of broadband current noise between the dynamic ($V_d$) and static ($V_s$) thresholds and changes to sliding of the crystal over a pinning barrier above the static threshold. This gives compelling

evidence for the Wigner crystal formation in these structures and shows the generality of the effect for different classes of strongly correlated two-dimensional electron systems. Applying a perpendicular magnetic field [4] promotes the double-threshold behavior to an order of magnitude lower voltages and considerably higher electron densities compared to the zero-field case. This indicates the stabilization of the quantum electron solid, which agrees with theoretical predictions.

# High-Energy Density Plasmas in the Laboratory Session 3

## Investigating the liquid-liquid, insulator-to-metal transition in hydrogen and deuterium

Marcus Knudson[1], Chad McCoy[1], Sakun Duwal[1], Kyle Cochrane[1], Heath Hanshaw[1], Martin Preising[2], Armin Bergermann[2], Michael Desjarlais[1], Ronald Redmer[2]

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The shock-ramp platform on the Sandia Z Accelerator enables off-Hugoniot experiments and allows access to a much wider region of phase space. In particular, this technique can produce relatively cool (~1-2 kK), high pressure (>300 GPa), high compression states (~10-15 fold compression) states, where hydrogen is predicted to undergo a first-order phase transition from an insulating molecular-like liquid to a conducting atomic-like liquid. In this talk we will survey the various theoretical predictions for the liquid-liquid, insulator-to-metal transition in hydrogen, discuss past experiments performed to investigate this transition, and present the results of recent experiments on both hydrogen and deuterium that extend these measurements to higher temperatures and lower pressures. We will also place these low-temperature and high-density measurements in context with metallization observed along the Hugoniot at much higher temperature and lower density, and dynamic conductivity measurements performed in the 1990s at intermediate temperature and density. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

## Visualizing laser-driven shocks in inertial fusion foams with high-resolution X-ray Free Electron Laser measurements

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Wetted foam capsules have been proposed for the delivery of nuclear fusion fuel in laser-driven inertial confinement fusion research and for the study of future inertial fusion power plant scenarios. While the foam structure will wick and hold the liquid hydrogen isotopes at cryogenic temperatures, the physical properties of the foam polymer material will need to be well understood under high-pressure conditions to make accurate predictions of fusion capsule implosion performance. Here, we are employing X-ray probing capabilities with unprecedented spatial resolution of 200 nm and temporal resolution of 50 fs to test our predictive modeling capabilities needed for advancing the field. Importantly, we aim to develop experimental capabilities that fire at high repetition rates to deliver data needed for stockpile stewardship research and will further benefit the development of nascent inertial fusion power efforts.

Our experiments at the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory have successfully observed streaming instabilities driven by high-intensity laser-irradiation of solid targets; these experiments visualize the subsequent launch and propagation of shock waves in the gigabar pressure regime and resolve the final adiabatic expansion and spalling of targets. These studies were recently extended measuring shock waves into aerogel foams and two-photon polymerization lattice foams providing shock speeds and densities from X-ray attenuation thus providing new equation of state data. Further, experiments have begun to directly measure the temperature with X-ray scattering and X-ray fluorescence both enabled by the LCLS X-ray laser beam. It is the goal of our studies to deliver experimental data with unprecedented accuracy to determine the adiabat and the equation of state of wetted foams and to enable successful designs of inertial fusion capsule implosions.

This work is supported by the U.S. Department of Energy, Fusion Energy Sciences, under FWP 100182, FWP 100866, and by DOE, DE-SC0024882 IFE-STAR.

# Investigating the equation of state and diamond formation behavior of polylactic acid and cellulose acetate under planetary interior conditions

Philipp May[1], Zhiyu He[2], Benjamin Heuser[1], Michael Stevenson[1], Marie-Luise Herbert[1], Jonas Kuhlke[1], Björn Lindqvist[1], Julian Lütgert[1, 3], Chongbing Qu[1], Samuel Schumacher[1], Divyanshu Ranjan[1, 3], Johannes Rips[1], Tommaso Vinci[4], Alessandra Ravasio[4], Alessandra Benuzzi-Mounaix[4], Jan Vorberger[3], Anja Schuster[5], Dominik Kraus[1, 3]

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This study presents an equation of state for polylactic acid [PLA, $(C_3H_4O_2)_n$] and cellulose acetate [CA, $(C_{10}H_{16}O_8)_n$]. These are similar in elemental composition to the planetary ices (C-H-N-O mixtures) modeled to make up a majority of Uranus' and Neptune's interiors [1]. Using Doppler

velocimetry and optical pyrometry on dynamically shock compressed PLA and CA — and confirming results by matching in situ x-ray diffraction data to density functional theory molecular dynamics simulations — pressures from 0.05 to 5.5 Mbar were studied. Such Mbar pressures are predicted for Uranus' and Neptune's planetary ice layer [2], so our data provide a benchmark for further simulations, experiments and space missions.

At these pressures, carbon starts to de-mix and be compressed into diamond. This is predicted to occur in Uranus' and Neptune's planetary ice layer [3] and has previously been observed in the lab, using in situ x-ray diffraction on shock compressed plastics like polyethylene terephthalate [PET, $(C_{10}H_8O_4)_n$] [4]. This work confirms nanodiamond crystallite formation in single-shocked PLA and CA which both possess a unique C to $H_2O$ ratio and are also bioplastics, meaning they are made from renewable resources and are somewhat biodegradable [5, 6]. Our results show how nanodiamond yield is affected by pressure and choice of material (PLA, CA, PET). They are a step towards efficiently producing lab-grown nanodiamonds which are desirable for their promising applications, e.g. in medicine [7].

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# Accelerated Scientific Computing of High-Repetition Rate Material Characterizationfor Fusion and Microelectronics

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Warm dense matter (WDM) represents a highly excited state that lies at the intersection of solids, plasmas, and liquids and that cannot be described by equilibrium theories. The transient nature of this state when created in a laboratory, as well as the difficulties in probing the strongly coupled interactions between the electrons and the ions, make it challenging to develop a complete understanding of matter in this regime. In this work, by exciting isolated ∼8 nm copper nanoparticles with a femtosecond laser below the ablation threshold, we create uniformly excited WDM. Using photoelectron spectroscopy, we measure the instantaneous electron temperature and extract the electron-ion coupling of the nanoparticle as it undergoes a solid-to-WDM phase transition. By comparing with state-of-the-art theories, we confirm that the superheated nanoparticles lie at the boundary between hot solids and plasmas, with associated strong electron-ion coupling. This is evidenced both by a fast energy loss of electrons to ions, and a

strong modulation of the electron temperature induced by strong acoustic breathing modes that change the nanoparticle volume. This work demonstrates a new route for experimental exploration of the exotic properties of WDM.

# High-Energy Density Plasmas in the Laboratory Session 4

## An ab initio study of silicon dioxide in the warm dense matter regime

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Silicon dioxide is a key geophysical material but it is also a widely used reference material in shock experiments. During giant impacts and in high-power laser experiments, $SiO_2$ is exposed to very high pressures and temperatures up to several times $10^5$ K. In both cases, $SiO_2$ is first compressed along the Hugoniot curve and then experiences an isentropic release. In shock-experiments, it can also undergo a reshock towards even higher compression states. As a reference material it needs to be characterized under all of these conditions with a high accuracy.

In this presentation we will show results from quantum molecular dynamics simulations applied to $SiO_2$ up to 12 g/cm$^3$ and 5x10$^5$ K. From these simulations, we extracted the equation of state of SiO2 in this regime and compared it with several experiments ensuring its accuracy and its ability to serve as a reference EOS for impedance matching methods. We also explored structural and transport properties to be used in geophysical and hydrodynamic models.

## Inhibited Electron-Ion Equilibration and Bond Hardening in Warm Dense Gold

Travis Griffin[1], Daniel Haden[2], Hae Ja Lee[3], Eric Galtier[3], eric cunningham[3], Dimitri Khaghani[3], lennart Wollenweber[4], Ben Armentrout[3], carson convery[3], karen appel[4], luke fletcher[3], Sebastian goede[4], jerome hastings[3], jeremy iratcabal[1], emma mcbride[5], jacob molina[1], giulio Monaco[6], Landon Morrison[1], hunter Stramel[1], sameen yunus[3], ulf zastrau[4], Siegrfried glenzer[3], gianluca gregor[7], Dirk Gericke[8], Bob Nagler[3], thomas White[1]

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When a high-intensity laser strikes a solid target, it rapidly and preferentially heats the electrons over the ions, creating a highly non-equilibrium state[1,2]. These transient states provide a critical

testbed for validating quantum mechanical theories of electron-ion interactions, yet the mechanism and timescales of electron-ion equilibration remain poorly understood, partly due to the lack of reliable experimental diagnostics for direct ion temperature measurement. Previous methods have inferred ion temperatures from structural measurements, but these approaches falter in non-equilibrium systems[3] where bond strengths vary significantly with electron temperature[4-8]. To address this, we have developed a high-resolution X-ray scattering platform to directly measure the evolution of ion temperature following laser irradiation. By analyzing the quasi-elastic Rayleigh peak, whose width is governed by Doppler broadening, we directly determine the ion velocity distribution and, consequently, their temperature[9]. Our measurements reveal evidence of inhibited electron-ion equilibration in the most highly non-equilibrium states and unequivocally demonstrate bond hardening in thin polycrystalline gold samples under warm dense matter conditions.

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# Classical Charged Systems Session 2

## Charge regulation: Theory and Simulations

Yan Levin[1]

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We present a theory that enables us to calculate the effective surface charge of colloidal particles and to efficiently obtain titration curves for different salt concentrations and pH [1].
To explore the validity of the theory we have also developed a Monte Carlo approach for performing titration simulations in the canonical ensemble
[2]. The standard constant pH (cpH) simulation methods are intrinsically grand canonical, allowing us to study the protonation state of molecules only as a function of pH in the reservoir [2,3]. Due to the Donnan potential between a system and an (implicit) reservoir of a semi-grand canonical simulation, the pH of the reservoir can be significantly different from that of an isolated system, for an identical protonation state. The new titration method avoids this difficulty by using canonical

reactive Monte Carlo algorithm to calculate the protonation state of macromolecules as a function of the total number of protons present inside the simulation cell. To properly
treat the long range Coulomb force, we use Ewald summation method, showing the importance of the Bethe potential for calculating pH of canonical systems.
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## Propagation and interaction of solitary waves in large area, strongly coupled, 2D dusty plasmas

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Solitary waves in a single-layer dusty plasmas can be excited by applying voltage pulses to conducting wires stretched across the dust particle layer. If the wire is bare, planar waves with straight wavefronts are excited. If only a short portion of the wire is uninsulated, a semicircular wave pattern can be obtained. If two separate sections of the same wire are stripped of insulation, two circular waves can be launched forming crossing wavefronts as they propagate in the system. We have realized these experimental scenarios in our large area dusty plasma chamber with planar electrode options up to 16 inches in diameter at the Hypervelocity Impacts & Dusty Plasmas Lab at Baylor University. The experiments were performed at low gas pressures (between 1 and 8 Pa) to minimize wave dissipation. We present the results of particle tracking velocimetry analysis of the high-resolution video sequences, shedding light on the microscopic details of solitary wave propagation and wave interaction with obstacles and other waves. The measured density and velocity distributions are compared with theoretical predictions based on nonlinear wave theory.

Support for this work from the US Department of Energy, Office of Science, Office of Fusion Energy Sciences under awards DE-SC0024681, the National Science Foundation under award number PHY-2308743, and NASA Grant 20-EW20_2-0053.

# Developments in Theoretical Methods and Numerical Techniques Session 2

# Exchange-correlation free-energy density functionals: recent developments and applications

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*Ab initio* molecular dynamics (AIMD) simulations based on the free-energy density functional theory (DFT), in combination with the Kubo-Greenwood formulation for transport and optical properties, have proven to be the most successful approach for understanding warm-dense-matter (WDM) and high-energy-density (HED) plasmas across different temperature regimes. DFT requires approximations for the exchange-correlation (XC) energy density functional, which effectively takes into account many-body interaction effects. Currently, the vast majority of DFT simulations of WDM and HED plasmas use zero-temperature (ground-state) XC functionals without explicit temperature dependence, leading to the neglect of thermal XC effects and degrading the accuracy of predictions in the regime of $T/T_F \sim 0.5$. In this talk, we discuss recent advances in the development of XC free-energy density functionals (i.e., functionals with explicit temperature dependence), including the thermal meta-generalized gradient approximation. Incorporation of some exact finite-temperature constraints makes thermal XC functionals accurate and broadly predictive over the entire temperature range. Thermal XC functionals show a significant improvement in the accuracy of DFT simulations for hydrogen and helium equations of state, as demonstrated by the comparison to the reference path-integral Monte Carlo data. Some other applications, including direct large-scale AIMD simulations of $H_2$/H-He mixtures at extreme conditions for accurate predictions of the demixing, insulator-metal transition, and miscibility boundaries are discussed as well. This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0004144 and US National Science Foundation PHY Grant No. 2205521.

# An Internally Consistent Model for High Energy Density Material Properties

Stephanie Hansen[1], Alina Kononov[1], Andrew Baczewski[1], Kelsey Adler[1], Lucas Stanek[1], Christopher Jennings[1]

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High energy density (HED) plasma systems such as giant planets, stars, and inertial confinement fusion (ICF) targets span an enormous range of material conditions, traversing extreme temperatures, densities, and pressures. Predictive hydrodynamic simulations of these plasma systems rely on atomic-scale models to generate and tabulate constitutive data such as equations of state (EOS), transport coefficients, and opacities. The HED community has developed a wide variety of models that can accurately calculate subsets of the needed data, but very few of these models can produce all required properties. Tables based on multiple models for different properties and/or different regimes are likely to have internal inconsistencies. In this talk,

we describe an average-atom model based on Kohn-Sham density functional theory (KS-DFT) that can predict a wide range of plasma properties, including detailed opacity and emissivity spectra with self-consistent line shapes. The predictions of the model are compared against benchmark-quality models such as time-dependent multi-center DFT and state-of-the-art collisional-radiative kinetics model. We then explore the impact of adopting these internally consistent constitutive data sets on the performance of magneto-inertial fusion targets.

This work was supported by SNL's LDRD program. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

## Inverse two-sided Laplace transform in quantum many-body theory:\\ generalized framework and the PyLIT open-source code base

Thomas Chuna[1, 2], Alexander Benedix-Robles[1, 2, 3], Phil-Alexander Hofmann[1, 2], Tobias Dornheim[1, 2], Michael Hecht[1, 2]

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In this work we provide model-free estimates of the dynamic structure factor for strongly coupled finite temperature electron liquids at coupling strength as high as $\Gamma \approx 154$. To do this, we analytically continue Path integral Monte Carlo (PIMC) Imaginary time correlation functions to the real frequency domain. This amounts to solving the notoriously ill-posed inverse Laplace transform. Despite numerous attempts, no universally accepted approach has been identified to solve this problem and many methods remain unsatisfactory. We propose an alternative physics-motivated formulation of the problem that improves the conditioning, expressing the DSF as a linear combination of kernels that satisfy physical properties of the DSF. We regularize our new problem formulation with a Bayesian prior of the DSF and investigate the commonly used entropic regularizer, as well as unexplored regularizers (\textit{i.e.}, the Wasserstein distance and the squared deviation from Bayesian prior). We compare our result to other approaches finding we are able to resolve a double roton-like feature in the electron liquid dispersion relation. As a key outcome, we developed the open-source Python library PyLIT (\textbf{Py}thon \textbf{L}aplace \textbf{I}nverse \textbf{T}ransform).

# Non-Equilibrium Systems Session 1

## Nonequilibrium Coulomb Systems

Dirk Gericke[1]

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Nonequilibrium processes are often essential for the study of strongly coupled Coulomb systems. They naturally occur during the creation of such matter in the laboratory and the relaxation toward equilibrium can highlight specific properties, like damping rates or the mode structure, that are hard to probe otherwise. The relaxation usually establishes both a new spatial arrangement and a new momentum distribution with times scales that strongly depend on the species considered. Moreover, the energy transfer between different species can be very complex and usually defines the time when a local thermal equilibrium is established.

This talk will review the relaxation processes in dense plasmas and warm dense matter. Special emphasis will be given to the influence of the potential energy and its relation to the new spatial arrangement. Moreover, theoretical concepts will be compared to experimental data wherever possible. The talk will follow the natural order of processes from the initial excitation to local thermal equilibrium. Thus, nonequilibrium electrons, including changes of the band occupation and ionisation, will be discussed first. Unfortunately, most comparisons of theoretical predictions and experimental data for these processes are rather indirect, e.g.~via the conductivity or optical properties.

Still, basic concepts can nowadays be tested. Secondly, the nuclear response will be considered. As the relaxation of the ions is often related to a phase change, it permits to observe well-pronounced thresholds directly.

The final focus of the talk will be on electron-ion temperature relaxation.

Recently, considerable progress has been made here theoretically, using first-principle simulations and towards precision measurements. Many of these results point to significant slower temperature equilibration than standard models predict. The underlying physics, an interplay of kinematics and collective excitations, highlights the complex dynamics in strongly coupled Coulomb systems.

## X-Ray Thomson Scattering from dense non-equilibrium plasmas using X-ray Free Electron Lasers

Luke Fletcher[1], Lex Andersen[1], Siegfried Glenzer[1], Jerry Hastings[1], Willow Martin[1], Iris Kunz[1], Madison Singleton[1], Emma McBride[2], Adrien Descamps[2], Sebastian Goede[3], Ulf Zastrau[3], Pawel Ordyna[4], Thomas Kluge[4], Martin Rehwald[4], Karl Zeil[4], Thomas Gawne[4], Tobias Dornheim[4], Peihao Sun[5]

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Recent advancements in X-ray Thomson scattering (XRTS) diagnostics, coupled with the ultra-fast and ultra-bright nature of X-ray Free Electron Lasers (XFELs), have significantly enhanced our ability to study dense plasmas under non-equilibrium conditions. These combined capabilities provide a unique experimental platform necessary for probing transient phenomena with unprecedented spatial and temporal resolution. Here we present two complementary

experimental approaches that leverage these technological developments. First, we use the energy-resolved scattering of X-ray pulses from a cryogenic hydrogen jet approximately 1 picosecond after irradiation with a fs-laser near intensities of $1\times10^{18}$ W/cm² to measure non-equilibrium hydrogen plasmas at electron temperatures approaching Te=400 eV. This platform enables direct observation of the generated high energy electron populations, providing fundamental insights into ionization dynamics and energy partition mechanisms. Second, we utilize SACLA's unique two-color mode to conduct X-ray pump-probe studies of mid-Z elements. Using two X-ray pulses (9.4 keV pump, 7 keV probe) with tunable fs-time delays, we precisely investigate electron thermalization dynamics in solid-density Ni and Cu targets. The pump pulse deposits energy selectively above the K-edge, while the probe pulse captures the subsequent electronic response with femtosecond precision. Both platforms implement stochastic spectroscopy alongside high-resolution spectrometers, dramatically enhancing spectral resolution and signal-to-noise. This innovative approach overcomes traditional limitations in XRTS measurements, enabling detection of ev-scale spectral features previously masked by instrument response functions. By measuring collective and non-collective scattering across sub-picosecond time delays, we establish a comprehensive understanding of electron thermalization before ionic energy transfer or hydrodynamic expansion occur. The temporal evolution of electron temperature, ionization state, and density can be directly measured, allowing for direct comparison to existing theoretical models. These experiments represent significant progress in understanding ultrafast energy transfer mechanisms in dense matter, with important implications for inertial confinement fusion, laboratory astrophysics, and planetary science.

# Temperature Measurements in Shocked Iron around the Melt with High-Resolution Inelastic X-ray Scattering

Bob Nagler[1]

[1]SLAC National Accelerator Laboratory

Given the prominence of iron in terrestrial planetary interiors, accurate and precise measurements of its physical properties is crucial for geophysics. In particular, the melting point of iron is still hotly debated at the conditions of the Earth’s interior.

We will show results of a very recent LCLS experiment that aimed to directly measure the temperature in shock-melted iron in a model-independent way, using high-resolution spectrally resolved x-ray scattering. In backscattering geometry, the photon Rayleigh peak is determined by the Doppler shift of the X-rays scattering from the ions in the melt. Due to the particle velocity and temperature behind the shock front, the Rayleigh peak will shift and broaden. In combination with diffraction data and VISAR, we can measure the temperature , pressure, and structure factor of the molten iron at conditions relevant to Earth’s interior and planetary science.

This method to determine temperature using high resulation IXS has been used before in combination X-ray Diffraction to determine unambigously the change in bond stregth in gold, which we will briefly discuss.

## Ultrafast electron thermalization and structural changes in laser-excited graphene studied by ab-initio approaches

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Intense ultrafast-laser pulses induce extreme non-equilibrium conditions in matter. In particular, most of the laser energy is absorbed by the electrons. The ensuing thermalization behavior in the electronic system from the induced highly non-equilibrium state is of utmost importance in understanding how materials behave when exposed to high-intensity lasers. This work explores how real-time Time-Dependent Density Functional Theory can thermalize electronic states and how those thermal states are represented. Using the Octopus code, we investigate how monolayer graphene behaves under laser excitation. We also calculate the distribution of occupations over time by projecting time-evolved wavefunctions onto ground-state wavefunctions. We look at the nature of thermalization in TDDFT by comparing how close this distribution comes to resembling the Fermi-Dirac distribution over time. Our results contribute to a deeper understanding of energy transport in two-dimensional materials under high-energy-density conditions by providing insight into the timescales and mechanisms governing thermalization in graphene. After the electron-equilibration process, the electronic system is traditionally described within density functional theory in the canonical ensemble ($N,V,T_e$) by a constant temperature and Mermin's functionals. Combining the findings of both methods allows us to determine a transition point between them. However, the assumption of an infinite heat bath coming from the laser has its limits, which leads to the question whether the highly excited electronic system is not best described theoretically in the microcanonical ensemble (N,V,E) assuming a constant entropy. Here, we compared ab initio molecular dynamics simulations obtained by describing electrons either in the canonical ensemble or by the microcanonical ensemble, as implemented in CHIVES. Our results for graphene indicate that laser-induced phenomena remain conceptually the same for low- and medium-strong excitations, after which the atoms follow the same microscopic pathways independent of the ensemble choice. At elevated intensities, the selection of the ensemble results in distinct structural changes.

# Dense and Astrophysical Plasmas Session 1

## Dynamic response properties in atomistic dense plasma

Alexander White[1]

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Time-dependent density functional theory (TD-DFT) has become a vital tool for modelling electronic response properties including electronic conductivity, stopping power and inelastic Xray Thomson Scattering. We have utilized a combination of traditional, orbital-free, and stochastic TD-DFT approaches to calculate these properties in dense plasmas. We will present a

comparison of orbital-free and Kohn-Sham approaches to calculate inelastic XRTS and demonstrate the critical role of nonadiabatic kinetic energy functionals, based on the homogeneous electron gas dynamic response function, which introduce dissipation. We will also present novel applications of TD-DFT to calculate the nonadiabatic Born effective charges / group conductivity and the nonadiabatic electron-ion coupling. The prior allows for a unique decomposition of the electronic optical response into ion groups, *e.g.* ions of the same element, while the latter provides a means of calculating equilibration rates in two temperature plasma.

## Material Properties of Saturn's Interior from Ab Initio Simulations

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Calculation of material properties from ab inito simulations along Jupiter [1] and Brown Dwarf adiabats [2] have been subject of earlier studies. However, accurate models of Saturn's interior are still very challenging. A recent study by Mankovich and Fortney on Jupiter and Saturn models was based on a single physical model [3] which predicts a strongly differentiated helium distribution in Saturn's deep interior, resulting in a helium-rich shell above a diffuse core.

We focus on the calculation of material properties of matter at P-T conditions along the Saturn model proposed by Mankovich and Fortney.

The dissociation of hydrogen as well as the onset of the helium-rich layer have profound impact on material properties: Dissociation of hydrogen triggers the metallization of the hydrogen sub-system and the band gap of the system closes. It also leads to negative values for the Thermal Expansion Coefficient α, promoting a stably stratified layer inside Saturn. The helium rain promotes another stably stratified layer above an almost pure He layer.

We present results on thermodynamic and transport properties of a hydrogen-helium-water mixture that closely resembles the element distribution of the Saturn model. We discuss implications of the results on our understanding of Saturn's interior and evolution.

## Estimating ionization states and continuum lowering from ab initio path integral Monte Carlo simulations for warm dense hydrogen

Hannah Bellenbaum[1,2], Maximilian Böhme[3], Michael Bonitz[4], Tilo Döppner[3], Luke Fletcher[5], Thomas Gawne[1,2], Dominik Kraus[6], Zhandos Moldabekov[1,2], Sebastian Schwalbe[1,2], Jan Vorberger[1], Tobias Dornheim[1,2]

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Warm dense matter (WDM) is a complex state of matter found in astrophysical environments and inertial confinement fusion, where ionization degree and continuum lowering play a crucial role but remain challenging to diagnose experimentally. In this work, we introduce a new approach to extracting these quantities for hydrogen by analyzing exact path integral Monte Carlo (PIMC) simulations using a chemical model based on the Chihara decomposition. Unlike direct experimental measurements, which often suffer from noise and model dependencies, PIMC simulations provide high-fidelity data under well-defined thermodynamic conditions. We employ a forward-fitting procedure, commonly used in x-ray Thomson scattering (XRTS) analysis, by fitting the dynamic structure factor (DSF) of the Chihara model to PIMC data across a broad range of densities, temperatures, and scattering wave vectors. This enables us to extract estimates for both ionization potential depression (IPD) and ionization state. We compare these extracted values against widely used models. Furthermore, by analyzing estimates across a wide range of scattering angles, we demonstrate the decreasing sensitivity of the DSF with respect to both IPD and ionization degree for increasing scattering angles in an XRTS experiment. Lastly, by applying the chemical model to exact PIMC data, we gain qualitative insights into the physics encoded in the imaginary-time correlation function (ITCF) and refine our understanding of structure factors obtained from quantum Monte Carlo simulations. This work establishes a pathway for validating chemical models against first-principles data, enhancing the accuracy of WDM diagnostics and advancing our theoretical description of dense plasmas.

# Crystal Nucleation in Dense White Dwarf Plasmas

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Little is known about the dynamics of crystallization in strongly coupled multicomponent plasmas. We use unbiased molecular dynamics, seeded molecular dynamics, and metadynamics simulations to calculate the free energy surface associated with the formation of small crystals in a bulk single-component Coulomb plasma. From this free energy, we can understand the rate that crystals form from the liquid as well as the distribution of small crystallites before complete solidification. Calculations of binary and ternary mixtures are applicable to white dwarf stars because the star's cooling rate depends on details the energy released during crystallization of the dense plasma mixtures in its core.

This material is based upon work supported by the Department of Energy National Nuclear Security Administration University of Rochester National Inertial Confinement Program under Award Number DE-NA0004144.

LA-UR-25-23647

# Plasmas in Condensed Matter Session 1

## Electron gas and dense hydrogen: from ground state energies to phase diagrams

Markus Holzmann[1]

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Exactly 45 years ago, the ground state phase diagram of the fermion one component plasma (or jellium) has been calculated by quantum Monte Carlo methods [1]. Since then, quantum Monte Carlo calculations have been applied to describe high pressure hydrogen, as well as electronic structure in simple materials. Still, quantum Monte Carlo methods are affected by various sources of bias due to the fermion sign problem and limitations of system sizes, and the electron gas model has remained central in the development of new methods. I will give a brief overview over recent developments, methodological advances and results, focusing on jellium and high pressure hydrogen (at ambient and low temperatures).

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## Collective Modes in Coulomb Systems with Spin-Orbit Coupling

Carlos Sa de Melo[1]

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In 3D plasma physics, Coulomb gases possess density collective excitations called plasmons. However, in 1D, Coulomb gases can be described by Tomonoga-Luttinger Liquids, where spin-charge separation arises, leading to low- energy collective modes described by charge and spin density waves that propagate at different velocities. Inspired by investigations of Dirac, Majorana and Weyl fermions in the context of particle, condensed matter and atomic physics, we propose the emergence of helical boson modes that we call Weyl bosons, the bosonic cousins of Weyl fermions [1]. We show that these exotic excitations arise naturally in one-dimensional interacting Fermi gases, when spin-orbit coupling and Zeeman fields are present, through the mixing charge and spin degrees of freedom [1,2]. We obtain the phase diagram of chemical potential versus Zeeman fields for given spin-orbit coupling and interactions, showing regions where zero, one or two types of Weyl bosons exist. We find that, when two types of Weyl bosons emerge, they must propagate with different velocities. Furthermore, we show that the disappearance of any Weyl boson species is described by a topological quantum phase transition of the Lifshitz type, where the velocity of the disappearing Weyl boson vanishes, and the velocity of the surviving Weyl boson develops a cusp at the transition boundary. Lastly, to detect the existence of Weyl bosons, we propose measurements of the dynamical structure factor tensor

(charge-charge, charge-spin and spin-spin), where the energy dispersions, spectral weights and helicities of the emergent Weyl bosons may be experimentally extracted.

[1] “Emergence and Detection of Weyl Bosons in Fermi Systems with Long-Ranged Interactions”, Xiaoyong Zhang and C. A. R. Sá de Melo (in preparation, 2025).

[2] “Beyond spin-charge separation: Helical modes and topological quantum phase transitions in one-dimensional Fermi gases with spin-orbit and Rabi couplings”, Xiaoyong Zhang and C. A. R. Sá de Melo, arXiv:2405.20255v1.

## Response of solid matter to high-intensity irradiation with X-ray free-electron-laser pulses focused to nanometer spot size.

Beata Ziaja-Motyka[1]

[1]CFEL, DESY, Hamburg, Germany

In this talk, I discuss the response of solid materials to the impact of X-ray free-electron-laser pulses focused to a nm spot size. After introducing fundamental physical processes contributing to the strong, localized ionization on-going, few examples of experimental measurements and the respective theory predictions obtained for various solids exposed to X-ray pulses of intensity up to 10^19 W/cm^2 and focused to 7 nm -200 nm spot sizes are shown. This gives a basis for the following critical assessment of unique opportunities and challenges underway to controlling transitions induced by such intense X-ray pulses. Perspectives for practical applications are also presented.

Figure caption: Valence charge density distribution of diamond for the (110) plane. It was measured at different delay times after the irradiation of diamond with a high-intensity X-ray pulse (PRL 126,117403 (2021)).

## A Machine Learning Study of Properties of D2O up to 8 Million Kelvin from First Principles

Margaret Berrens[1], Sebastien Hamel[1], John Pask[1], Abhiraj Sharma[2]

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Accurately modeling dense plasmas across a broad range of pressure and temperature conditions presents a significant challenge, critical to enhancing our understanding of stellar and planetary physics, inertial confinement fusion and other high energy density experiments. Kohn-Sham density functional theory (DFT) is a commonly used method for studying materials with no empirical parameters. However, Kohn-Sham calculations of warm dense matter (WDM) present distinct challenges, one of which is the increase in the number of partially occupied states as the temperature rises where the cubic scaling bottleneck manifests itself at smaller system

sizes. This bottleneck is especially limiting in ab initio molecular dynamics (AIMD), where solving the Kohn-Sham equations hundreds of thousands of times may be necessary to access relevant timescales. The development of the Spectral Partition DFT method (SPDFT) is well suited for calculations at high temperature as only a small number of bands must be explicitely calculated.[1] While this method greatly reduces computational costs, it still involves substantial computational expenses in the context of molecular dynamics. This limitation can be overcome by machine learned force field (MLFF) schemes, in particular on-the-fly MLFF training during MD simulations bypasses the need to generate an extensive training dataset prior to generating the MLFF. The efficiency and efficacy of such a scheme has only recently been applied in the context of WDM.[2] In this study, we employ Spectral Partition DFT MD accelerated with an on-the-fly MLFF, to examine the properties of deuterated water ($D_2O$) under WDM conditions near the principal Hugoniot, going from ambient conditions, through the warm dense matter regime and into the plasma regime. We calculate the equation of state, Hugoniot, pair distribution functions, diffusion coefficients, and viscosity at densities ranging from 3.0 g/cm³ to 4.5 g/cm³ and temperatures from 10 kK to 8 MK using SPDFT method.

# Plasmas in Condensed Matter Session 2

## Quantum-Monte Carlo study of electron-hole bilayer at low-density

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Bilayer electron-hole systems provide a unique platform for investigating fundamental properties of excitons, particularly their condensation and superfluid behavior. By means of Quantum Monte Carlo we explore the formation and stability of interlayer excitons driven by Coulomb interactions as well as the appearance of the complexes made of excitons such as bi-exciton or quadri-exciton, for the system with valley degeneracy, and their effect on the exciton condensation.

Our focus will be on the low-density region of the system where the screening is reduced and the Coulomb interactions enhanced; if the repulsion between the well-formed elementary objects (excitons, biexcitons..) can become dominant over the kinetic energy, the spontaneus formation of a Wigner Crystal can occur.

## Universal neural wave functions for high-pressure hydrogen

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We leverage the power of neural quantum states to describe the ground state wave function of solid and liquid dense hydrogen, including both electronic and protonic degrees of freedom. For static protons, the resulting Born-Oppenheimer energies are consistently lower than all previous projector Monte Carlo calculations for systems containing up to 128 hydrogen atoms.

In contrast to conventional methods, we introduce a universal trial wave function whose variational parameters are optimized simultaneously over a large set of proton configurations spanning a wide pressure-temperature spectrum and covering both molecular and atomic phases. This global optimization not only yields lower energies compared to benchmarks but also brings an enormous reduction in computational cost.

By including nuclear quantum effects in the zero-temperature ground state, thus going beyond the Born-Oppenheimer approximation, our description overcomes major limitations of current wave functions, notably by avoiding any explicit symmetry assumption on the expected quantum crystal and sidestepping efficiency issues of imaginary time evolution with disparate mass scales. As a first application, we examine crystal formation in an extremely high-density region where pressure-induced melting is expected.

# Confined and Mesoscopic Coulomb Systems Session 2

## Excitons and polaritons in novel two-dimensional materials, embedded in a microcavity

Oleg Berman[1]

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It has been shown that when a graphene sheet is subject strain, electrons and holes behave as though they are in an external magnetic field. The quantum Hall effect for direct and indirect excitons was predicted in the monolayers and double layers of gapped graphene under strain-induced gauge pseudomagnetic fields, correspondingly [1].

We predict that, when coupled to a microcavity, excitons in strained graphene can form robust entangled states suitable for quantum information applications [2,3]. A Tavis-Cummings model describes the interactions between two [2] and more excitons [3] and a cavity mode. The study reveals that under specific conditions, entanglement can be protected from decay and even enhanced by dissipation, delivering promising insights for quantum computing technologies.

We proposed 2D materials-based time crystals (TCs). We analyzed the dynamics of exciton and polariton Bose-Einstein condensates (BECs) under a periodic potential [4]. We considered two such systems, the first consists of exciton-polaritons in a nanoribbon of transition metal dichalcogenides (TMDCs), within a curved microcavity, which serves as the source of the periodic potential. The second, made of bare excitons in a nanoribbon of twisted TMDC bilayer, which produces a periodic Moiré potential that can be controlled by the twist angle. We proved that such systems behave as semiclassical time crystals [4].

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# Confined and Mesoscopic Coulomb Systems Session 3

## Electron crystals in two-dimensional materials

Ilya Esterlis[1]

[1]University of Wisconsin - Madison

Recent experiments have demonstrated that quantum Wigner crystals—states of matter near zero temperature in which itinerant electrons spontaneously crystallize—are ubiquitous in the phase diagrams of two-dimensional materials, including graphene-based systems and atomically thin transition-metal dichalcogenides. These discoveries have opened new avenues for exploring the rich physics of Wigner crystals, including their magnetic properties, instabilities, and quantum melting. I will summarize key experimental findings to date and discuss theoretical proposals for novel magnetic and "metallic crystal" phases that may emerge in monolayer and bilayer electron crystals.

## Uncovering correlated phases in moiré materials: an ab initio approach to 2D continuum Hamiltonians

Yubo Yang[1]

[1]Hofstra University

Moiré materials offer a versatile platform for exploring strongly correlated electronic phases, yet conventional mean-field methods often fall short in capturing their complexity. Cooperation of many electrons over large spatial separations is a key ingredient in most of the unusual phenomena observed. However, theoretical calculations frequently discard electron correlation, the long-range nature of the electron-electron interactions, or both.

In this talk, I will present recent advances in solving interacting moiré continuum Hamiltonians using high-accuracy Quantum Monte Carlo techniques and machine learning-assisted wavefunction methods (Neural Quantum States). These approaches reveal rich and exotic correlated states, such as generalized Wigner crystal and ferromagnetic charge-density wave. They also provide predictions beyond the reach of standard approximations. I will emphasize connections between experiment and the theoretical model in exploring of how the theoretical framework and experimental findings can inform one another.

## Mapping of Sheath Electric field in Low-temperature Radio-frequency plasma using levitated dust grains.

Dinil Jose[1], Vedant Singh[1], Ravi Kumar[1], Ranganathan Gopalakrishnan[1]

[1]The University of Memphis

Electric field measurements in the sheath region are crucial in understanding the dynamics of dust grains. In capacitively coupled RF plasmas, the electric field above the powered electrode can influence the dust particles directly via the electrostatic force and indirectly through the ion drag force helping them form a two-dimensional dust cluster. Most dusty plasma experiments are performed at relatively low input powers (< 5 W using a 13.56 MHz radio frequency generator) and at higher neutral pressures (~20 to 200 mTorr). Diagnosing such weakly ionized, low-temperature plasmas can be challenging using existing in-situ probe techniques. In this study, inspired by the experimental method to measure sheath electric fields by A A Samarian (2005) [1], dust particles are used to infer the electric field in the sheath region. The response of dust particles to external laser perturbation contains information on the background electric field, particularly in the region where the dust clusters are formed. Trajectory simulations based on Langevin dynamics are employed with the obtained background electric field to generate both the crystal and liquid cluster data which can be compared directly with the experiments. The measurements using Langmuir and emissive probes and their limitations are also discussed.

This research is supported by the US Department of Energy FY2020 Early Career Award DE-SC0021106, Facilities Award DE-SC0023416 from the Office of Fusion Energy Science and US Army Research Office - Sciences of Extreme Materials Branch Award #W911NF-23-2-0013

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# 1 Minute Poster Talks

# Modeling the Equilibrium Alignment of Grains in Complex Plasma

Benny Rodriguez Saenz[1], Diana Jimenez Marti[1], Lorin Matthews[1], Truell Hyde[1]

[1]Baylor University

Modeling the Equilibrium Alignment of Grains in Complex Plasma

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In laboratory dusty plasma experiments, complex plasma (micron-sized particles that become charged and interact with their plasma environment) offers a unique platform for studying fundamental processes in strongly coupled plasmas. This work focuses on processes that affect the dynamics of non-symmetric grains immersed in a flowing ion environment. In nature, dust grains are typically irregular and non-spherical, and their asymmetry plays a crucial role in influencing how they interact with electromagnetic forces and plasma flows. Understanding these interactions is important for accurately interpreting natural phenomena, yet conducting experiments with naturally irregular grains presents significant challenges. Therefore, to make the investigation more feasible while still capturing essential dynamics, we model these non-spherical grains as aggregates of spherical monomers. Due to the presence of multiple forces acting on these aggregates, such as drag and electric forces, they experience different torques, ultimately reaching an equilibrium orientation with respect to the plasma flow. Our study employs simulations with aggregates of varying aspect ratios, from elongated to nearly spherical, to explore whether the final orientation can be predicted or characterized by intrinsic properties such as the electric dipole moment or geometric form. Understanding these relationships can provide deeper insight into the self-organization and dynamics of complex plasmas, which are relevant not only in laboratory conditions but also in astrophysical environments like planetary rings and interstellar clouds.

Support for this work from the US Department of Energy, Office of Science, Office of Fusion Energy Sciences under award number DOE DE-SC0024681 and National Science Foundation under award number PHY2308743 is gratefully acknowledged.

# Predicting the uniform electron gas stopping power at moderate and strong coupling

Saule Syzganbayeva[1], Alexey Filinov[2], Assel Ashikbayeva[1], Abdiadil Askaruly[1], Lazzat Yerimbetova[1], Manuel Barriga-Carrasco[3], Yuriy Arkhipov[1], Igor Tkachenko[4]

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We present a detailed study of the stopping power of a homogeneous electron gas in moderate and strong coupling regimes using the self-consistent version of the method of moments [1-5] as the key theoretical approach capable of expressing the dynamic characteristics of the system in terms of the static ones, which are the moments. We develop a robust framework, which relies on nine sum rules and other exact relationships to analyze electron-electron interactions and their impact on energy loss processes. We derive an expression for the polarizational stopping power that takes into account both quantum statistical and electron correlation effects. Our results demonstrate significant deviations from classical stopping power predictions [6-8] (see Fig.), especially under the strong coupling regime, when electron dynamics is highly dependent on the collective behavior presenting two collective modes, each of them interacting with the incoming projectile separately. This work not only advances the theoretical understanding of the uniform electron fluid but also has implications for practical applications in fields such as plasma physics and materials science.

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*Acknowledgements. This research was supported by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan under Grant #AP09260349 and Ministry of Science and Innovation, Spain, under Grant #PID2021-127381NB-I00.*

# The finite temperature 2D UEG: dielectric schemes and ab initio path integral Monte Carlo simulations

Fotios Kalkavouras[1], Panagiotis Tolias[1], Tobias Dornheim[2, 3], Jan Vorberger[3]

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There have been numerous advances in the description of the finite temperature 3D uniform electron gas (UEG) both in quantum Monte Carlo simulations [1,2] and in the self-consistent dielectric formalism [3,4,5]. Unfortunately, 2D UEG investigations have been limited to the ground state limit [6] with a near-absence of reliable results for the finite temperature 2D UEG [7]. Nevertheless, advances in semiconductor applications will likely require taking into account the electronic temperature in the future. We present extensive thermodynamic and structural results for the finite temperature 2D UEG within the self-consistent dielectric formalism. In particular, 2D

versions of the Singwi-Tosi-Land-Sjölander (STLS) scheme that is tailor made for weak-to-moderate coupling [8] and the hypernetted-chain (HNC) scheme that is tailor made for moderate-to-strong coupling [9] have been developed. Efficient numerical schemes have been devised for their accurate solution; the 2D-STLS scheme benefits from the emergence of complete elliptic integrals of the first and second kind, while the 2D-HNC scheme benefits from the use of the bipolar convolution theorem. A detailed comparison with new Path Integral Monte Carlo results is carried out.

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## Modeling the Sn Equation of State to Constrain the Liquid Vapor Dome

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The off-Hugoniot expanded states of matter remain poorly understood for several materials of interest to the national defense and planetary impact communities. Predictive modeling of phase transformations remains limited—specifically in the onset of vaporization in Sn under high-pressure conditions. To address this gap, we have developed an equation of state (EOS) model using the analytical modeling software ANEOS, which uses current expanded states data to predict the location of the liquid-vapor equilibrium region. This has allowed for a more comprehensive understanding of the thermodynamic behavior of Sn. Our equation of state has also enabled us to investigate Sn response to impacts with different materials in the 2D hydrocode simulation software, PyKO. Our model will help to inform the design of future planar impact experiments on our single stage and two stage light gas guns in order to best constrain the Sn equation of state.

## Measurement of interfacial thermal resistance in high-energy-density matter

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Heat transport throughout high-energy-density systems and across interfaces is a ubiquitous phenomenon with many unresolved aspects. In particular, thermal conductivity in warm dense matter has extensive theoretical predictions but lacks experimental benchmarking [1]. We use Fresnel diffractive radiography [2-4] to measure the interface evolution in an isochorically-heated plastic-coated tungsten wire. After pressure equilibration, the interface is hydrodynamically stable and its evolution is driven primarily through thermal conduction, which modifies the temperature and density profiles. We find experimental evidence of a significant and long-lasting thermal barrier between the warm dense tungsten and its surrounding plastic. This temperature jump is characteristically similar to temperature jumps resulting from interfacial thermal resistance [5], indicating that the phenomenon can play a significant role in these extreme conditions, despite an abundance of free electrons [6]. The restricted heat flow may be of particular importance for inertial confinement fusion experiments, where instability-prone material interfaces play a large role in determining capsule implosion performance [7].

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# Design of a Thomson parabola ion spectrometer for high-intensity short-pulse laser experiments at MEC

Andrea Zabala[1]

[1]SLAC National Accelerator Laboratory

In high-intensity laser-plasma interactions, characterizing ion species and their energy distributions is crucial for monitoring laser-matter interaction and understanding fundamental processes at the origin of laser acceleration of charged particles. At the Matter in Extreme Conditions (MEC) instrument of the Linac Coherent Light Source (LCLS), we are developing a Thomson Parabola Ion Spectrometer (TPS) specifically tailored for use with the short-pulse laser configuration. This diagnostic tool will allow for charge-resolved ion detection by utilizing combined electric and magnetic fields to deflect charged particles according to their charge-to-mass ratios and kinetic energy. The TPS is being designed for use in the MEC target chamber while taking into consideration the constraints of the optical laser and chamber dimensions. It will feature custom made micro-channel plate (MCP) stacks, boasting significant advantages, such as compatibility with high repetition rates and electromagnetic pulse (EMP) conditions. It will serve as a valuable tool for laser-plasma experiments, capable of measuring a wide range of accelerated ions. Current research is focused on calculating magnetic field guidelines to later perform trajectory simulations that will optimize the TPS design for implementation in upcoming experiments. This will enable more in-depth investigation of

parameters such as maximum ion energy under varying laser conditions and target materials. This project not only improves MEC's experimental capabilities but also provides a hands-on opportunity to apply principles of electromagnetism, charged particle optics, and detector physics in a high-impact research environment.

## Ion Temperature Measurements in Dense Compressed Solids

Michael Larsen[1], Thomas White[1], Travis Griffin[1], Daniel Haden[1], Hae Ja Lee[2], Eric Galtier[2], Eric Cunningham[2], Dimitri Khaghani[2], Lennard Wollenweber[3], Ben Armentrout[2], Carson Convery[2], Karen Appel[3], Luke Fletcher[2], Sebastian Goede[3], Jerome Hastings[2], Jeremy Iratcabal[1], Emma McBride[4], Jacob Molina[1,5], Giulio Monaco[6], Landon Morrison[1,7], Hunter Stramel[1], Sameen Yunus[2,8], Ulf Zastrau[3], Siegfried Glenzer[2], Gianluca Gregori[7], Dirk Gericke[9], Bob Nagler[2]

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Advancing our understanding of material behavior under extreme conditions is crucial for breakthroughs in geophysics, astrophysics, and shock physics. Central to this pursuit is the precise measurement of the equation of state (EOS), delineating how materials react to changes in temperature, pressure, and density. Yet the accurate determination of temperature - a pivotal element of EOS - poses significant challenges, especially in dense, opaque materials prevalent in dynamic compression studies. To address this gap, we have pioneered an approach utilizing high-resolution X-ray scattering technology at free-electron laser facilities. The inelastic X-ray scattering at millielectronvolt energies (meV-IXS) platform leverages a monochromatic X-ray source to penetrate dense matter, allowing us to measure the ion temperature. In backscattering geometry at high temperatures, we observe Doppler broadening of the Rayleigh peak, providing a model-independent assessment of temperature through the ion velocity distribution. However, for highly compressed solids that remain below the melt temperature, the presence of phonons complicates the analysis. In this work, we use multi-phonon calculations and molecular dynamic simulations to investigate how X-ray scattering spectra relate to ion temperature for solid matter.

## Rotons and ghost plasmons in multicomponent ionic mixtures

Abdiadil Askaruly[1], Assel Ashikbayeva[1], Askar Davletov[1], Saule Syzganbayeva[1], Lazzat Yerimbetova[1], Ivan Pirogov[1], Alexey Filinov[2], Arkhipov Yuriy[1], Igor Tkachenko[3]

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Dynamic properties of two important examples of multicomponent ionic mixtures are studied using the self-consistent version of the method of moments [1, 2, 3]. Partial radial distribution functions of $H^+$ - $D^+$ $D^+$-$T^+$-$^3He^{++}$ mixtures determined in the modified HNC approximation are employed within the to determine the poles and zeros of the inverse dielectric function of the mixtures. It is determined that in a $H^+$ - $D^+$ mixture the lifetime of the roton branch of the system plasmon-roton mode is comparable or even shorter than the mode period, i.e., that this branch is virtual or strongly decaying. In the ternary mixture $D^+$-$T^+$-$^3He^{++}$ this branch's decrement is found to be smaller than its frequency, so that it becomes observable. The form of the calculated dynamic structure factors confirms these results. Conditions are established for the mixture dielectric function to lose its analyticity in the complex frequency upper half-plane [4, 5], and the relative contributions to the *f* -sum rule of the unique pole located on the positive part of the imaginary axis called the "ghost plasmon" and of other two poles located in the lower half-plane are found. In Fig. circles and diamonds stand for the real and imaginary parts of the plasmon-roton mode, and squares correspond to the imaginary parts of the dielectric function pole on the complex frequency upper half-plane.

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# Anisotropic electric potential of dust filaments

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Dust particles within the Plasmakristall-4 (PK-4) facility on board the International Space Station (ISS) have been observed to form extended filaments when exposed to a DC polarity-switched electric field. These filaments align in the direction of the applied electric field. Along this direction, the particles are strongly coupled, forming structures that resemble crystalline filaments. In contrast, the system shows liquid-like behavior in the transverse direction due to the weaker coupling between particles across the filaments. The presence of dust particles alters both the charge distribution and the spatial potential distribution within the plasma, leading to regions of positive and negative potential. The anisotropic coupling in these dusty plasmas can be

compared with numerical simulations to investigate anisotropies in the potential distribution near these filaments. These variations depend on factors such as interparticle distance, pressure, dust density, and more. In this work we simulate the charging of dust chains using an N-body numerical simulation of dust and ions for several plasma conditions. Results are used to develop a potential model which reproduces the effect of the dust and ion wakes potential in the region near dust chains. The resulting effective potential will be used to model dust dynamics and compare to those observed in the PK-4 experiment.

Support for this work from the US Department of Energy, Office of Science, Office of Fusion Energy Sciences under awards DE-SC0021334 and DE-SC0024681, the National Science Foundation under award numbers PHY-1740203,PHY-2308742 and PHY-2308743, NSF EPSCoR FTPP OIA-2148653 and NVIDIA Corporate Applied Research Program is gratefully acknowledged. All authors acknowledge the joint ESA/Roscosmos Experiment Plasmakristall-4 (PK-4) onboard the International Space Station.

## Foundations of magnetohydrodynamics

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A derivation of magnetohydrodynamics (MHD) valid beyond the usual ideal gas approximation is presented. Non-equilibrium thermodynamics, a macroscopic framework for describing irreversible processes, is used to obtain conservation equations and linear constitutive relations. When coupled with Maxwell's equations, this provides closed fluid equations in terms of material properties of the plasma, described by the equation of state and transport coefficients. It is then shown how these properties are connected to microscopic dynamics using the Irving-Kirkwood procedure and Green-Kubo relations. Discussions of symmetry arguments and the Onsager-Casimir relations are provided, which allow one to vastly simplify the number of independent coefficients. Importantly, expressions for current density, heat flux, and stress (conventionally Ohm's law, Fourier's law, and Newton's law) take different forms in systems with a non-ideal equation of state. The traditional form of the MHD equations, which is usually obtained from a Chapman-Enskog solution of the Boltzmann equation, corresponds to the ideal gas limit of the general equations.

This work was supported by the US National Science Foundation under Grant No. PHY-2205506.

## Extracting the same information from dynamics structure factors and imaginary time correlation function

Thomas Chuna[1,2], Nicholas Barnfield[3], Jan Vorberger[2], Michael Friedlander[4], Tim Hoheisel[5], Zhandos Moldabekov[1,2], Panagiotis Tolias[6], Alexander Robles[1,2,7], Phil Hofmann[1,2], Michael Hecht[1,2], Tobias Dornheim[1,2]

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For many years, the analytic continuation of imaginary time correlation functions have challenged the scientific community. The analytic continuation amounts to an inverse Laplace transform of a function with poles. In theory, the Laplace transform, like the Fourier transform, is a one to one mapping so the same information is present in either representation. However, in practice the inversion is difficult. In this work, we present new investigations that have applied analytic continuation tools to observe the same phenomena in both the imaginary and real time. We focus on observing a repeated roton (i.e. double roton) structure [submission in progress], differentiating which pair potential was used in PIMC simulation [https://arxiv.org/abs/2504.00737], and the satisfaction of sum rules https://arxiv.org/pdf/2503.20433]. Note that in the analytic tools there are no constraints enforcing these phenomena. For these three phenomena, we have find good agreement between real time and imaginary time representations.

# High Energy Density Science Opportunities at Lawrence Livermore National Laboratory

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Lawrence Livermore National Laboratory has many exciting opportunities for students, postdoctoral scholars, research scientists, and faculty. The High Energy Density Science (HEDS) Center facilitates connections across the research community, accelerating efforts to establish new collaborations where experts can share their knowledge, and early-career investigators can receive the mentoring they need to be ready to solve tomorrow’s problems and shape the future of HEDS. We have vibrant summer student programs, mini-courses, seminars, prestigious postdoctoral fellowships, and a mini-sabbatical program for faculty. Our employees and collaborators may obtain access to state-of-the-art facilities, including the National Ignition Facility, Jupiter Laser Facility, high performance computing, and the HEDS Technology Facility. Come learn about these opportunities and how to join our community.

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

# Comparing finite-temperature and zero-temperature models in the strong interaction limit

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Density functional theory, a widely used quantum mechanical method, has been a powerful tool in simulating high-temperature processes such as fusion reactions conducted at the National Ignition Facility. The thermal upside-down adiabatic connection is a formalism that smoothly connects the physical system at a specific density to a fictitious infinitely interacting (strictly correlated) reference system via a scaling factor. This method yields an exact expression for the decorrelation free energy, the missing piece needed to calculate the total free energy of the realistically interacting system. While this technique is well established at zero temperature, further work is needed to apply this method to finite-temperature systems. This work probes the use of zero-temperature methods as well as newly derived thermal counterparts for calculating decorrelation free energies at finite temperatures. By exploring the behavior of this new derivation over a range of temperatures, we evaluate the usefulness of this method for modeling experimental processes.

# Measuring Interfacial Thermal Resistance in HED Matter

Damien Batayeh[1], Thomas White[1], Sarah Shores Prins[1], Otto Landen[2], Dirk Gericke[3], Yuan Ping[2], Matthew Oliver[1, 4], Tilo Doeppner[2], Laurent Divol[2], Gregory Kemp[2], Markus Schoelmerich[2, 5], Wolfgang Theobald[6], Phil Sterne[2], Nathaniel Shaffer[6], Christopher Spindloe[4], Nils Brouwer[7], Landon Morrison[1], Cameron Allen[1, 8]

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Heat transport in high-energy-density systems, particularly in warm dense matter, remains a complex and largely unverified area of study. Using Fresnel Diffractive Radiography, we investigated the interface evolution in an isochorically heated plastic-coated tungsten wire. Following pressure equilibration, the interface remained hydrodynamically stable, with heat transfer primarily governed by thermal conduction, shaping the temperature and density profiles. Our results indicate the presence of a persistent thermal barrier between warm dense tungsten and the surrounding plastic, consistent with interfacial thermal resistance despite the abundance of free electrons. This restricted heat flow has significant implications for inertial confinement fusion, where material interface stability is crucial in implosion performance. Furthermore, the presence of fluorine introduced uncertainty in determining the equation of state, and the unexpectedly high thermal conductivity observed may be influenced by its presence. A more controlled analysis using pure CH plastic could provide further clarity on these effects.

# Ionization and Partition Function Regularization in Multicomponent Warm Dense Matter

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The study of warm dense matter (WDM) is crucial for understanding extreme physical environments, such as the interiors of astrophysical objects, nuclear explosions, and inertial confinement fusion experiments. It is known that WDM exhibits unique properties distinct from both classical gases and condensed matter, making it a key focus of both fundamental and applied research. A major challenge in this field is the development of accurate theoretical models capable of describing matter under such extreme conditions.

Computational modeling plays a vital role in WDM research, bridging gaps in experimental data. In contrast. this study employs a generalized chemical model for multicomponent systems that allows for the derivation of analytical expressions for the composition and thermodynamic properties of the medium. A key advantage of this model is its flexibility in incorporating an arbitrary number of components and any type of interaction potentials in the Helmholtz free energy, and thereby enabling unified treatment of diverse problems.

A significant issue addressed herein is the divergence of the internal partition function for composite particles in the ideal gas approximation. In our approach, each excited state is treated as a distinct species with a single energy level. The inclusion of interparticle interactions enables the identification of critical quantum numbers beyond which level populations vanish.

Unlike traditional methods of truncating the partition function, the proposed approach naturally excludes states whose excitation energies exceed the ionization potential lowering (IPL). These states are no longer physically relevant as they transition into the continuum. The IPL from excited levels is calculated by minimizing the total Helmholtz free energy, allowing the determination of the threshold at which excited states become delocalized.

# Thermal Conductivity and Shock Ringing in Warm Dense Matter

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The performance of inertial confinement fusion (ICF) implosions is highly dependent on the transport properties of the materials involved, but experimental data for these properties remains sparse. This is largely due to the inherent difficulty in probing matter at high energy densities (HED), and has lead to a reliance on numerical modelling to quantify material properties at these conditions. However, predictions of transport properties are not well constrained, with order-of-magnitude variations between models even for well-studied materials at the same densities and temperatures. Here we present our latest progress in developing a method to infer the thermal conductivity of ablator materials in multi-layer targets irradiated by a high-energy laser. In such geometries, reverberating compression waves arise from the impedance gradients at material boundaries; using a Spitzer-Hãrm conduction model, we find that the amplitude and length scale of these waves are strongly coupled to material thermal conductivities. This opens up the possibility of constraining simulated conductivities in ICF-relevant materials at HED conditions by using x-ray imaging to measure shock ringing experimentally. We present preliminary results for Kapton using data from void collapse experiments at the Linac Coherent Light Source (LCLS), and find conductivities that are within an order of magnitude of existing models.

# Advancing diagnostic capabilities for warm-dense matter on the National Ignition Facility

David Bishel[1], Maximilian Boehme[1], Stanislav Stoupin[1], Michael MacDonald[1], Veronika Kruse[1], Justin Buscho[1], Tilo Doeppner[1], Tobias Dornheim[2], Hannah Bellenbaum[2], Dominik Kraus[3], Johannes Rips[3], Luke Fletcher[4], Siegfried Glenzer[4], Dirk Gericke[5]

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X-ray scattering is a powerful diagnostic for characterizing warm-dense matter, as it simultaneously encodes details of electron correlations, ionization, and the plasma thermodynamic state [S. H. Glenzer and R. Redmer, Rev. Mod. Phys. 81, 1625 (2009).] However, scattering measurements from laser-driven samples must contend with not only a short-lived and rapidly evolving state but also weak scattering cross-sections. A continuous scattering measurement would provide unprecedented access to the ion-plasma interaction while also characterizing the evolving thermodynamic state. To provide the required diagnostic capability, we have designed a high-efficiency x-ray spectrometer coupled to a streak camera for use on the National Ignition Facility. The spectrometer utilizes a conically curved crystal to increase solid angle collection and to sagitally focus the signal onto the 1-mm wide streak camera slit. The resulting continuous record enables reconstruction of the full experiment history from a single experiment, not only increasing data collection per experiment by a factor of five relative to existing spectrometers [T. Döppner, et al., Rev. Sci. Instrum. 85 (2014)] but also eliminating the uncertainty introduced by combining data from multiple shots. Two applications will be discussed: improved constraint of pressure-induced electron delocalization in implosions [T. Döppner, et al., Nature 618, 270 (2023)] and temperature diagnosis of doubly-shocked foams [M. J. MacDonald, et al., Phys. Plasmas 30 (2023)].

This work was performed under the auspices of the U.S. Department of Energy and an appointment to the Office of Science, by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

# Electrical conductivity and reflectivity of HCNO mixtures at planetary interior conditions

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[1]LULI

About two thirds of known exoplanets are classified as super−Earths and mini−Neptunes due to their similar size compared to their Solar System cousins. To date, it remains unclear if similar−sized exoplanets share a complementary composition of their interiors. Insights from atomic scale simulations are therefore key in moving forward. In particular electrical conductivity and reflectivity derived from density functional theory molecular dynamics (DFT-MD) simulations have proven useful to connect material property results from shock-compression experiments to planetary models [1-3].

This presentation provides an overview of the recent advances made in the study of ice-rich giant planets such as Uranus and Neptune by investigating the electronic properties of HCNO mixtures. We calculate electrical conductivities and reflectivities of dynamically compressed water, ammonia and their mixtures with DFT-MD [4,5]. The influence of the exchange-correlation functional on the results is examined in detail. Our findings indicate that the consistent use of the HSE hybrid functional reproduces experimental results much better than the commonly used PBE functional. Finally, we present a comparison of our results to new shock-compression data.

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# Towards a fully self-consistent embedding theory average atom model for warm dense hydrogen

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Accurate models of warm dense matter are challenging to produce without invoking computationally expensive methods to describe the electronic and ionic interactions. Density functional theory (DFT)-based average atom models (AAM) reduce the complex ionic many-body system to a spherical average over local environments or charge states. This approach significantly reduces computation time while still retaining fair accuracy in evaluating equations of state, mean ionizations, and more. Despite their success, DFT-based AAMs struggle to fully capture all electronic interactions, since they rely on averaging over detailed density distributions. One particular contribution in dense plasma environments is the effect of overlapping electron densities between neighboring atoms, which alters orbital kinetic energies due to enforced orthogonality. To address this contribution, we have developed a self-consistent average atom model that includes these interactions via the non-additive kinetic potential $V^{NAD}$ as in DFT embedding theories. $V^{NAD}$ can be computed using Thomas-Fermi, von Weizsäcker, or more sophisticated finite-temperature free energy functionals. The model takes as input an ion-ion pair correlation function, $g_{II}(r)$—such as calculated from fully quantum mechanical treatments like quantum molecular dynamics—which encodes the plasma properties such as density and temperature. It then solves for a fully self-consistent electronic subsystem, including $V^{NAD}$, based on the ionic configuration given by $g_{II}(r)$. This framework introduces $V^{NAD}$ as a novel interaction term in existing AAMs and enables the inclusion of interactions beyond the central atom. We have applied this model to hydrogen at solid density and temperatures of a few eV, investigating the impact of $V^{NAD}$ on electron densities, energy shifts, and mean ionization.

This work was supported by the U.S. Department of Energy, National Nuclear Security Administration, Minority Serving Institution Partnership Program, under Award DE-NA0003984. And with computing resources from Pinnacles (NSF MRI, # 2019144) at University of California, Merced.

# An experimental platform for investigation of shock waves in MG magnetic fields

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The Zebra pulsed power generator at UNR produces magnetic fields of 1-3 MG with rod and coil loads. We developed an experimental platform to study shock waves in strong magnetic fields. Shock waves were studied in hydrogen, argon, and nitrogen media provided by the gas jet. A Leopard laser pulse with a 1ns duration and energy of 10-20 J was focused on copper rod loads.

The azimuthal magnetic field near the focus was 1-2 MG. Laser diagnostics included end on interferometry and shadowgraphy at wavelengths of 532 nm and 266 nm and a 4-frame side on diagnostics at 532nm. We present visualization of shock waves and the dynamics of shock waves in hydrogen in the magnetic field. The magnetic field extends the shock front along the magnetic field lines. A velocity of some shock waves exceeds 2000km/s.

## Measuring the Thermal Conductivity of Iron Alloys Near Planetary Core Conditions at the OMEGA Laser Facility

Sarah Shores Prins[1], Cameron Allen[1,2], Laurent Divol[3], Ryan Enoki[1], Dirk Gericke[4], Landon Morrison[1,5], Matthew Oliver[6], Yuan Ping[3], Nathaniel Shaffer[7], Jaya Sicard[1,3], Christopher Spindloe[6], Tilo Doeppner[3], Thomas White[1]

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Understanding the thermal conductivity of materials found in the cores of rocky planets can help us predict planetary evolution and understand the mechanisms necessary for the existence of organic life. However, significant variations in scientific modeling and a scarcity of experimental measurements limit our understanding of materials at the extremes of temperature and pressure. We propose to use our isochoric heating platform developed for the OMEGA 60 Laser System to recreate the conditions close to those found in the interiors of Earth-like planets. We will subject a 5 μm Fe/Ni (95/5 %wt) alloy wire (representing an iron planetary core) with a 10 μm borosilicate glass encasing (representing the silicate mantle) to planetary core conditions. After pressure equilibration, the shape of the density profile across the Fe95/Ni5-glass interface evolves primarily through thermal conductivity. This profile will be measured with a spatial resolution on the order of 1 μm, in line with previous work[1,2,3]. This will enable the accurate extraction of the conductivity scale length, which in turn will be used to validate competing theoretical models.

## Utilizing Stochastic Correlation Spectroscopy for High Resolution X-Ray Scattering from Warm Dense Matter

Lex Andersen[1], Luke Fletcher[1], Willow Martin[1,2], Siegfried Glenzer[1], Jerry Hastings[1], Madison Singleton[1], Emma McBride[3], Adrien Descamps[3], Sebastian Goede[4], Ulf Zastrau[4], Peihao Sun[5], Iris Kunz[1]

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Warm Dense Matter (WDM) presents a unique challenge for theoretical modelling due to both ion-ion interactions and partially degenerate electrons being present. As current condensed

matter theory and plasma physics theory are inadequate for predicting WDM conditions, implementing high resolution stochastic correlation x-ray spectroscopy will provide accurate measurements of electron temperature and average ionization with an improved signal-to-noise ratio. This diagnostic uses the correlation of individual incident, non-monochromatized SASE pulses and the corresponding X-ray Thomson scattering (XRTS) to reconstruct the full dynamic structure factor. Requiring an accurate measurement of the incoming free electron laser, we construct a single shot hard X-ray spectrometer with a flat silicone crystal which yields results that are spatially and spectrally uniform. Initially measuring the collective forward scattering of cold aluminum at European XFEL, we demonstrate eV-scale resolution, benchmarking our results with multi-component scattering simulations (MCSS). Stochastic Correlation Spectroscopy is being fielded at SACLA, taking advantage of the two color modes to pump and probe at two unique photon energies. By analyzing isochorically heated copper and nickel in the WDM regime, we hope to provide accurate plasma parameters and low signal-to-noise XRTS to constrain plasma modelling parameters.

## Estimates of the dynamic structure factor for the finite temperature electron liquid via analytic continuation of path integral Monte Carlo data

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Path integral Monte Carlo (PIMC) simulations are one of the few methods which can describe the structure of the plasma in Warm Dense Matter. However, the imaginary time correlation functions (ITCF) estimated by PIMC simulations must be analytically continuated back to real time to extract dynamic information about the system. One of the most ubiquitous approaches to analytic continuation is the maximum entropy method (MEM). The MEM is typically used with Bryan's controversial algorithm [Rothkopf, "Bryan’s Maximum Entropy Method" Data 5.3 (2020)]. We investigate a dual Newton optimization algorithm to be used within the MEM that addresses known issues. We pay special attention to our uncertainty providing analytic bounds for the algorithm's error as well as numerical estimates of the uncertainty arising from both the ITCF and the regularization weight. We use the MEM to investigate authentic PIMC data for the uniform electron gas and further substantiate the roton-type feature in the dispersion relation. This work demonstrates that the all-purpose maximum entropy method can reliably estimate the DSF from PIMC data and establishes a path towards model-free estimates of the DSF in ion-electron systems.

# Inverse Supersymmetry in Finite Temperature Bose-Fermi Mixtures

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We investigate near-supersymmetric Bose-Fermi mixtures at temperatures greater than the condensation temperature of the constituent bosons. In this regime, we describe the breaking of supersymmetry (SUSY) between bosons and fermions with up to two internal states through the emergence of fermionic Goldstino modes. We draw a distinction between typical SUSY, where bosons have pseudospin 0 and fermions have pseudospin 1/2, and inverse supersymmetry (iSUSY), where bosons have pseudospin 1/2 and fermions have pseudospin 0. We highlight that the Goldstino pseudospin is carried by either its constituent fermion (SUSY) or boson (iSUSY). We then distinguish between these two cases by depicting their differing effects on the spectral function of the fermionic atomic species. Lastly, we propose an RF-spectroscopy measurement, analogous to momentum (angular) resolved photoemission in condensed matter physics, to measure the pseudospin-dependent spectral function.

# Ion Temperature Measurements in High Energy Density Liquids

Brittany Callin[1], Thomas White[1], Michael Larsen[1], Travis Griffin[1]

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The equation of state (EOS) is fundamental in understanding the dynamics of materials under extreme conditions. Having a complete EOS of high energy density (HED) matter is important in astrophysics, geophysics, and shock physics. Many techniques exist to access density and pressure, but measuring ion temperature remains particularly challenging. We have developed a new technique using meV X-ray scattering at free electron lasers that is able to access ion temperature through measurement of the dynamic structure factor. In the ideal gas limit the dynamic structure factor can be approximated as a Gaussian through the Maxwell-Boltzmann distribution. Using Molecular Dynamic simulations, we can test the validity of the Gaussian form of the dynamic structure factor in high energy density liquids. The limit at which the ideal gas limit is a valid model is dependent on the coupling parameter (Γ), the screening parameter (κ), and the wavenumber k.

## Neural Quantum States for Two-Dimensional Materials

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I'll present recent work using Variational Monte Carlo (VMC) with expressive neural network ansatze. We first study a moire system by modeling a two-dimensional electron gas (2DEG) in a honeycomb potential. In our simulations, we find a novel and highly correlated state at a low filling of one electron for every four minima which we refer to as a paired Wigner crystal. This is similar to the molecular Wigner crystals recently observed in twisted bilayer tungsten disulfide. In contrast to these, however, the paired Wigner crystal occurs with fewer electrons than minima. Then, we'll turn our attention to the 2DEG without a moire potential but with impurities and study this system with a similar neural network ansatz. This is motivated by a recent experiment studying the 2DEG with an improved STM resolution that allows us to determine the location of impurities and model their effect in VMC. By assuming they are trapped electrons with screened and unscreened Coulomb interactions, we find excellent agreement between VMC and experiment then provide further analysis to characterize the system.

## Particle-in-Cell Simulations of Laser-Driven Gold (Au) Targets

Olivia Stinson[1]

[1]slac

Proton acceleration via laser-plasma interactions offers a powerful alternative to traditional ion accelerators, providing compact systems capable of delivering high-energy ion beams critical for applications in cancer therapy and inertial confinement fusion (ICF). A recent experimental study using ultra-thin gold foils irradiated by the NePTUN laser system revealed a sharp increase in proton energies, attributed to the onset of relativistically induced transparency (RIT). This regime allows the laser to penetrate deeper into the target and sustain acceleration over longer timescales, enhancing efficiency beyond what is predicted by traditional Target Normal Sheath Acceleration (TNSA) models. In this work we explore the role of target design in optimizing focused ion acceleration. We study the relationship between target thickness and electron refluxing with 1D and 2D particle-in-cell (PIC) simulations.

## Theoretical perspectives on the stability and phase transitions of $MgO_2$ at Earth's mantle conditions

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Magnesium and oxygen are two of the most abundant elements in terrestrial planets, and their compounds—especially MgO—form the foundation of planetary mantle models. However, the high oxygen fugacity in planetary mantles can possibly form superoxides that have O stoichiometries higher than MgO. Understanding the extreme condition behavior of these Mg-superoxides can thus improve our understanding of their composition, seismic behavior, and thermal evolution of the oxygen-rich mantles of Earth-like exoplanets.

The present work specifically focuses on understanding the high pressure and high temperature behavior of $MgO_2$. Although thermodynamically unstable at ambient conditions, past crystal structure searches performed at 0 K has indicated that $MgO_2$ can be stable above 116 GPa till ~600 GPa [1]. Further, static compression experiments using diamond anvil cells have indicated that $MgO_2$ can become thermodynamically stable at pressures above ~96 GPa till 2150 K [2].

In the present study, we investigate the temperature-dependent dynamical stability of $MgO_2$ at ~100 GPa using first-principles phonon calculations within the quasi-harmonic approximation coupled with the anharmonicity from the density-functional theory (*DFT*) based molecular dynamics (*MD*) simulations. We analyze the phonon dispersion relations of different solid phases of $MgO_2$ across a wide pressure-temperature range to identify regions where the structure remains dynamically stable. Using the *DFT-MD* simulations, we further extend our understanding of possible phase transitions including melting of $MgO_2$ in our *P-T* conditions of interest. We expect the present results on the high-pressure phase stability of $MgO_2$ can have important impacts in high energy density sciences and planetary sciences.

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# Diffusion Coefficients of Warm Dense Water

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We investigate the phase-dependent diffusion behavior of water under extreme conditions using first-principles molecular dynamics simulations. Mean square displacements are analyzed to extract diffusion coefficients for hydrogen and oxygen in the liquid, solid, and superionic regimes. The results provide insight into ionic mobility across phase boundaries and are relevant for understanding water-rich planetary interiors. Particular emphasis is placed on identifying the onset of superionicity and the suppression of diffusion in the solid state.

# Roadmap to frequency dependent opacities from DFT-MD simulations

Isleydys Silva Torrecilla[1], Armin Bergermann[1], Maximilian Boehme[2]

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The frequency-dependent opacities of materials under extreme conditions play a central role in the interpretation of astrophysical observations and the design of high-energy-density experiments. In this work, we compute the dielectric function and resulting opacities of warm dense hydrogen using density function theory but also time-dependent density functional theory. We combine low-frequency intraband contributions—relevant for transport properties—with high-energy interband transitions, which dominate XUV and soft X-ray absorption. This two-step approach enables a consistent treatment of both metallic and bound-electron effects across a wide frequency range.

# On-the-fly machine learning studies of nickel in Mars core conditions

Maitrayee Ghosh[1], Arianna Gleason-Holbrook[1], Siegfried Glenzer[1]

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The warm dense matter (WDM) conditions - characterized by gigapascal pressures and few thousands of Kelvin temperature, are observed in the planetary interiors. Besides experimental techniques, atomistic simulations, particularly based on density-functional theory (DFT), play a key role in elucidating the microscopic properties in the WDM regime. However, accurate DFT-molecular dynamics (MD) suffer from major limitations of small cell sizes (up to 500-1000 atoms), few picoseconds of simulation, and high computational cost.

In this presentation, we demonstrate the use of density-functional theory coupled with on-the-fly machine learning strategy, as implemented in the Vienna *ab initio* Simulation Package (VASP) [1, 2], to overcome the finite size limitations of DFT. This approach dynamically trains a machine-learned force field (MLFF) during the simulation, allowing the model to bypass computationally expensive DFT calculations when sufficient accuracy has been achieved, thereby accelerating the overall computation [3].

We focus on nickel that has high abundance in the cores of small terrestrial planets like Mars and Venus. Despite multiple experiments and theoretical simulations, a consensus on the melt curve data at high pressure high temperature conditions still lacks for nickel. With our MLFF based simulations involving over 16,000 atoms of face-centered cubic (fcc) nickel, our melt temperatures align with experimental results using the void mediated nucleation approach. Our elastic constant calculations further indicates that fcc nickel is elastically anisotropic, further exhibited in the directional anisotropy in sound velocities. Our results demonstrate the

effectiveness of ML-accelerated simulations in extending the reach of pure *ab initio* simulations to larger scales for modeling complex material behaviors in planetary core conditions.

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3. Jinnouchi *et al.* **Phys. Rev. B**, 100 (1), 014105, 2019.


## A statistical approach to Stark broadening for complex ions


Kelsey Adler[1]

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Lineshapes encode a wealth of information about the plasmas that produce them, including plasma composition, density, temperature, motion and rotation, and magnitude of electric and magnetic fields. In particular, Stark broadening encodes information about the electric microfields generated by neighboring ions in a plasma and is a valuable density diagnostic. Producing lineshapes for complex atoms with 3 or more active electrons using standard perturbation theory can have prohibitively high computational costs. We present a simple and computationally straightforward heuristic model that can be used for ions of any complexity. Our statistical approach uses transition energies, energy shifts, and radial density distributions from a self-consistent average atom code to produce Stark-broadened lineshapes. We present comparisons to standard line-broadening methods for lines from one-and two-electron aluminum ions.


# Poster Session

## An experimental platform for investigation of shock waves in MG magnetic fields


Zach Minaker[1], Vladimir Ivanov[1], Roberto Mancini[1], Thomas White[1]

[1]University of Nevada, Reno



The Zebra pulsed power generator at UNR produces magnetic fields of 1-3 MG with rod and coil loads. We developed an experimental platform to study shock waves in strong magnetic fields. Shock waves were studied in hydrogen, argon, and nitrogen media provided by the gas jet. A Leopard laser pulse with a 1ns duration and energy of 10-20 J was focused on copper rod loads. The azimuthal magnetic field near the focus was 1-2 MG. Laser diagnostics included end on interferometry and shadowgraphy at wavelengths of 532 nm and 266 nm and a 4-frame side on

diagnostics at 532nm. We present visualization of shock waves and the dynamics of shock waves in hydrogen in the magnetic field. The magnetic field extends the shock front along the magnetic field lines. A velocity of some shock waves exceeds 2000km/s.

## Particle-in-Cell Simulations of Laser-Driven Gold (Au) Targets

Olivia Stinson[1]

[1]slac

Proton acceleration via laser-plasma interactions offers a powerful alternative to traditional ion accelerators, providing compact systems capable of delivering high-energy ion beams critical for applications in cancer therapy and inertial confinement fusion (ICF). A recent experimental study using ultra-thin gold foils irradiated by the NePTUN laser system revealed a sharp increase in proton energies, attributed to the onset of relativistically induced transparency (RIT). This regime allows the laser to penetrate deeper into the target and sustain acceleration over longer timescales, enhancing efficiency beyond what is predicted by traditional Target Normal Sheath Acceleration (TNSA) models. In this work we explore the role of target design in optimizing focused ion acceleration. We study the relationship between target thickness and electron refluxing with 1D and 2D particle-in-cell (PIC) simulations.

## Modeling the Equilibrium Alignment of Grains in Complex Plasma

Benny Rodriguez Saenz[1], Diana Jimenez Marti[1], Lorin Matthews[1], Truell Hyde[1]

[1]Baylor University

Modeling the Equilibrium Alignment of Grains in Complex Plasma

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In laboratory dusty plasma experiments, complex plasma (micron-sized particles that become charged and interact with their plasma environment) offers a unique platform for studying fundamental processes in strongly coupled plasmas. This work focuses on processes that affect the dynamics of non-symmetric grains immersed in a flowing ion environment. In nature, dust grains are typically irregular and non-spherical, and their asymmetry plays a crucial role in influencing how they interact with electromagnetic forces and plasma flows. Understanding these interactions is important for accurately interpreting natural phenomena, yet conducting experiments with naturally irregular grains presents significant challenges. Therefore, to make the investigation more feasible while still capturing essential dynamics, we model these non-spherical grains as aggregates of spherical monomers. Due to the presence of multiple forces acting on these aggregates, such as drag and electric forces, they experience different torques, ultimately reaching an equilibrium orientation with respect to the plasma flow. Our study employs

simulations with aggregates of varying aspect ratios, from elongated to nearly spherical, to explore whether the final orientation can be predicted or characterized by intrinsic properties such as the electric dipole moment or geometric form. Understanding these relationships can provide deeper insight into the self-organization and dynamics of complex plasmas, which are relevant not only in laboratory conditions but also in astrophysical environments like planetary rings and interstellar clouds.

Support for this work from the US Department of Energy, Office of Science, Office of Fusion Energy Sciences under award number DOE DE-SC0024681 and National Science Foundation under award number PHY2308743 is gratefully acknowledged.

## Foundations of magnetohydrodynamics

Jarett LeVan[1], Scott Baalrud[1]

[1]NERS, University of Michigan, Ann Arbor, United States of America

A derivation of magnetohydrodynamics (MHD) valid beyond the usual ideal gas approximation is presented. Non-equilibrium thermodynamics, a macroscopic framework for describing irreversible processes, is used to obtain conservation equations and linear constitutive relations. When coupled with Maxwell's equations, this provides closed fluid equations in terms of material properties of the plasma, described by the equation of state and transport coefficients. It is then shown how these properties are connected to microscopic dynamics using the Irving-Kirkwood procedure and Green-Kubo relations. Discussions of symmetry arguments and the Onsager-Casimir relations are provided, which allow one to vastly simplify the number of independent coefficients. Importantly, expressions for current density, heat flux, and stress (conventionally Ohm's law, Fourier's law, and Newton's law) take different forms in systems with a non-ideal equation of state. The traditional form of the MHD equations, which is usually obtained from a Chapman-Enskog solution of the Boltzmann equation, corresponds to the ideal gas limit of the general equations.

This work was supported by the US National Science Foundation under Grant No. PHY-2205506.

## Anisotropic electric potential of dust filaments

Diana Jimenez Marti[1], Benny Rodriguez Saenz[1], Bradley Andrew[2], Brooks Howe[2], Lorin Matthews[1], Truell Hyde[1], Evdokiya Kostadinova[2], Luca Guazzotto[2]

[1]Baylor University, [2]Auburn University

Dust particles within the Plasmakristall-4 (PK-4) facility on board the International Space Station (ISS) have been observed to form extended filaments when exposed to a DC polarity-switched electric field. These filaments align in the direction of the applied electric field. Along this direction, the particles are strongly coupled, forming structures that resemble crystalline filaments. In contrast, the system shows liquid-like behavior in the transverse direction due to the weaker

coupling between particles across the filaments. The presence of dust particles alters both the charge distribution and the spatial potential distribution within the plasma, leading to regions of positive and negative potential. The anisotropic coupling in these dusty plasmas can be compared with numerical simulations to investigate anisotropies in the potential distribution near these filaments. These variations depend on factors such as interparticle distance, pressure, dust density, and more. In this work we simulate the charging of dust chains using an N-body numerical simulation of dust and ions for several plasma conditions. Results are used to develop a potential model which reproduces the effect of the dust and ion wakes potential in the region near dust chains. The resulting effective potential will be used to model dust dynamics and compare to those observed in the PK-4 experiment.

Support for this work from the US Department of Energy, Office of Science, Office of Fusion Energy Sciences under awards DE-SC0021334 and DE-SC0024681, the National Science Foundation under award numbers PHY-1740203,PHY-2308742 and PHY-2308743, NSF EPSCoR FTPP OIA-2148653 and NVIDIA Corporate Applied Research Program is gratefully acknowledged. All authors acknowledge the joint ESA/Roscosmos Experiment Plasmakristall-4 (PK-4) onboard the International Space Station.

# Ion Temperature Measurements in High Energy Density Liquids

Brittany Callin[1], Thomas White[1], Michael Larsen[1], Travis Griffin[1]

[1]University Of Nevada, Reno

The equation of state (EOS) is fundamental in understanding the dynamics of materials under extreme conditions. Having a complete EOS of high energy density (HED) matter is important in astrophysics, geophysics, and shock physics. Many techniques exist to access density and pressure, but measuring ion temperature remains particularly challenging. We have developed a new technique using meV X-ray scattering at free electron lasers that is able to access ion temperature through measurement of the dynamic structure factor. In the ideal gas limit the dynamic structure factor can be approximated as a Gaussian through the Maxwell-Boltzmann distribution. Using Molecular Dynamic simulations, we can test the validity of the Gaussian form of the dynamic structure factor in high energy density liquids. The limit at which the ideal gas limit is a valid model is dependent on the coupling parameter (Γ), the screening parameter (κ), and the wavenumber k.

# Measuring Interfacial Thermal Resistance in HED Matter

Damien Batayeh[1], Thomas White[1], Sarah Shores Prins[1], Otto Landen[2], Dirk Gericke[3], Yuan Ping[2], Matthew Oliver[1, 4], Tilo Doeppner[2], Laurent Divol[2], Gregory Kemp[2], Markus Schoelmerich[2, 5], Wolfgang Theobald[6], Phil Sterne[2], Nathaniel Shaffer[6], Christopher Spindloe[4], Nils Brouwer[7], Landon Morrison[1], Cameron Allen[1, 8]

[1]University of Nevada, Reno, [2]LLNL, [3]University of Warwick, [4]STFC, [5]PSI, [6]LLE, [7]European XFEL, [8]LANL

Heat transport in high-energy-density systems, particularly in warm dense matter, remains a complex and largely unverified area of study. Using Fresnel Diffractive Radiography, we investigated the interface evolution in an isochorically heated plastic-coated tungsten wire. Following pressure equilibration, the interface remained hydrodynamically stable, with heat transfer primarily governed by thermal conduction, shaping the temperature and density profiles. Our results indicate the presence of a persistent thermal barrier between warm dense tungsten and the surrounding plastic, consistent with interfacial thermal resistance despite the abundance of free electrons. This restricted heat flow has significant implications for inertial confinement fusion, where material interface stability is crucial in implosion performance. Furthermore, the presence of fluorine introduced uncertainty in determining the equation of state, and the unexpectedly high thermal conductivity observed may be influenced by its presence. A more controlled analysis using pure CH plastic could provide further clarity on these effects.

# Comparing finite-temperature and zero-temperature models in the strong interaction limit

Sage Gorney[1], Vincent Martinetto[1], Brittany Harding[1], Aurora Pribram-Jones[1]

[1]University of California, Merced

Density functional theory, a widely used quantum mechanical method, has been a powerful tool in simulating high-temperature processes such as fusion reactions conducted at the National Ignition Facility. The thermal upside-down adiabatic connection is a formalism that smoothly connects the physical system at a specific density to a fictitious infinitely interacting (strictly correlated) reference system via a scaling factor. This method yields an exact expression for the decorrelation free energy, the missing piece needed to calculate the total free energy of the realistically interacting system. While this technique is well established at zero temperature, further work is needed to apply this method to finite-temperature systems. This work probes the use of zero-temperature methods as well as newly derived thermal counterparts for calculating decorrelation free energies at finite temperatures. By exploring the behavior of this new derivation over a range of temperatures, we evaluate the usefulness of this method for modeling experimental processes.

# Electrical conductivity and reflectivity of HCNO mixtures at planetary interior conditions

Mandy Bethkenhagen[1], Léon Andriambariarijaona[1], Alessandra Benuzzi-Mounaix[1], Tommaso Vinci[1], Alessandra Ravasio[1]

[1]LULI

About two thirds of known exoplanets are classified as super−Earths and mini−Neptunes due to their similar size compared to their Solar System cousins. To date, it remains unclear if similar−sized exoplanets share a complementary composition of their interiors. Insights from atomic scale simulations are therefore key in moving forward. In particular electrical conductivity and reflectivity derived from density functional theory molecular dynamics (DFT-MD) simulations have proven useful to connect material property results from shock-compression experiments to planetary models [1-3].

This presentation provides an overview of the recent advances made in the study of ice-rich giant planets such as Uranus and Neptune by investigating the electronic properties of HCNO mixtures. We calculate electrical conductivities and reflectivities of dynamically compressed water, ammonia and their mixtures with DFT-MD [4,5]. The influence of the exchange-correlation functional on the results is examined in detail. Our findings indicate that the consistent use of the HSE hybrid functional reproduces experimental results much better than the commonly used PBE functional. Finally, we present a comparison of our results to new shock-compression data.

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# Extracting the same information from dynamics structure factors and imaginary time correlation function

Thomas Chuna[1, 2], Nicholas Barnfield[3], Jan Vorberger[2], Michael Friedlander[4], Tim Hoheisel[5], Zhandos Moldabekov[1, 2], Panagiotis Tolias[6], Alexander Robles[1, 2, 7], Phil Hofmann[1, 2], Michael Hecht[1, 2], Tobias Dornheim[1, 2]

[1]Center for Advanced Systems Understanding (CASUS), [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), [3]Harvard University, [4]University of British Columbia, [5]McGill University, [6]Space and Plasma Physics, Royal Institute of Technology (KTH), [7]Technische Universit\"at  Dresden

For many years, the analytic continuation of imaginary time correlation functions have challenged the scientific community. The analytic continuation amounts to an inverse Laplace transform of a function with poles. In theory, the Laplace transform, like the Fourier transform, is a one to one mapping so the same information is present in either representation. However, in practice the inversion is difficult. In this work, we present new investigations that have applied analytic continuation tools to observe the same phenomena in both the imaginary and real time. We focus on observing a repeated roton (i.e. double roton) structure [submission in progress], differentiating which pair potential was used in PIMC simulation [https://arxiv.org/abs/2504.00737], and the satisfaction of sum rules https://arxiv.org/pdf/2503.20433]. Note that in the analytic tools there are no constraints enforcing these phenomena. For these three phenomena, we have find good agreement between real time and imaginary time representations.

## High Energy Density Science Opportunities at Lawrence Livermore National Laboratory

Paul Grabowski[1]

[1]Lawrence Livermore National Laboratory

Lawrence Livermore National Laboratory has many exciting opportunities for students, postdoctoral scholars, research scientists, and faculty. The High Energy Density Science (HEDS) Center facilitates connections across the research community, accelerating efforts to establish new collaborations where experts can share their knowledge, and early-career investigators can receive the mentoring they need to be ready to solve tomorrow’s problems and shape the future of HEDS. We have vibrant summer student programs, mini-courses, seminars, prestigious postdoctoral fellowships, and a mini-sabbatical program for faculty. Our employees and collaborators may obtain access to state-of-the-art facilities, including the National Ignition Facility, Jupiter Laser Facility, high performance computing, and the HEDS Technology Facility. Come learn about these opportunities and how to join our community.

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

## Towards a fully self-consistent embedding theory average atom model for warm dense hydrogen

Sameen Yunus[1], David Strubbe[1]

[1]University of California, Merced

Accurate models of warm dense matter are challenging to produce without invoking computationally expensive methods to describe the electronic and ionic interactions. Density functional theory (DFT)-based average atom models (AAM) reduce the complex ionic many-body system to a spherical average over local environments or charge states. This approach significantly reduces computation time while still retaining fair accuracy in evaluating equations of state, mean ionizations, and more. Despite their success, DFT-based AAMs struggle to fully capture all electronic interactions, since they rely on averaging over detailed density distributions. One particular contribution in dense plasma environments is the effect of overlapping electron densities between neighboring atoms, which alters orbital kinetic energies due to enforced orthogonality. To address this contribution, we have developed a self-consistent average atom model that includes these interactions via the non-additive kinetic potential $V^{NAD}$ as in DFT embedding theories. $V^{NAD}$ can be computed using Thomas-Fermi, von Weizsäcker, or more sophisticated finite-temperature free energy functionals. The model takes as input an ion-ion pair correlation function, $g_{II}(r)$—such as calculated from fully quantum mechanical treatments like quantum molecular dynamics—which encodes the plasma properties such as density and temperature. It then solves for a fully self-consistent electronic subsystem, including $V^{NAD}$, based on the ionic configuration given by $g_{II}(r)$. This framework introduces $V^{NAD}$ as a novel interaction term in existing AAMs and enables the inclusion of interactions beyond the central atom. We have applied this model to hydrogen at solid density and temperatures of a few eV, investigating the impact of $V^{NAD}$ on electron densities, energy shifts, and mean ionization.

This work was supported by the U.S. Department of Energy, National Nuclear Security Administration, Minority Serving Institution Partnership Program, under Award DE-NA0003984. And with computing resources from Pinnacles (NSF MRI, # 2019144) at University of California, Merced.

## Neural Quantum States for Two-Dimensional Materials

Conor Smith[1], Shiwei Zhang[1]

[1]Flatiron Institute

I'll present recent work using Variational Monte Carlo (VMC) with expressive neural network ansatze. We first study a moire system by modeling a two-dimensional electron gas (2DEG) in a honeycomb potential. In our simulations, we find a novel and highly correlated state at a low filling of one electron for every four minima which we refer to as a paired Wigner crystal. This is similar to the molecular Wigner crystals recently observed in twisted bilayer tungsten disulfide. In contrast to these, however, the paired Wigner crystal occurs with fewer electrons than minima. Then, we'll turn our attention to the 2DEG without a moire potential but with impurities and study this system with a similar neural network ansatz. This is motivated by a recent experiment studying the 2DEG with an improved STM resolution that allows us to determine the location of impurities and model their effect in VMC. By assuming they are trapped electrons with screened

and unscreened Coulomb interactions, we find excellent agreement between VMC and experiment then provide further analysis to characterize the system.

## A statistical approach to Stark broadening for complex ions

Kelsey Adler[1]

[1]Sandia National Laboratories

Lineshapes encode a wealth of information about the plasmas that produce them, including plasma composition, density, temperature, motion and rotation, and magnitude of electric and magnetic fields. In particular, Stark broadening encodes information about the electric microfields generated by neighboring ions in a plasma and is a valuable density diagnostic. Producing lineshapes for complex atoms with 3 or more active electrons using standard perturbation theory can have prohibitively high computational costs. We present a simple and computationally straightforward heuristic model that can be used for ions of any complexity. Our statistical approach uses transition energies, energy shifts, and radial density distributions from a self-consistent average atom code to produce Stark-broadened lineshapes. We present comparisons to standard line-broadening methods for lines from one-and two-electron aluminum ions.

## Rotons and ghost plasmons in multicomponent ionic mixtures

Abdiadil Askaruly[1], Assel Ashikbayeva[1], Askar Davletov[1], Saule Syzganbayeva[1], Lazzat Yerimbetova[1], Ivan Pirogov[1], Alexey Filinov[2], Arkhipov Yuriy[1], Igor Tkachenko[3]

[1]Department of Physics and Technology, IETP, al-Farabi Kazakh National University, Almaty, Kazakhstan, [2]Christian-Albrechts-Universitat zu Kiel, Kiel, Germany, [3]Departamento de Matemática Aplicada, Universitat Politècnica de València, Valencia, Spain

Dynamic properties of two important examples of multicomponent ionic mixtures are studied using the self-consistent version of the method of moments [1, 2, 3]. Partial radial distribution functions of $H^+$ - $D^+$ $D^+$-$T^+$-$^3He^{++}$ mixtures determined in the modified HNC approximation are employed within the to determine the poles and zeros of the inverse dielectric function of the mixtures. It is determined that in a $H^+$ - $D^+$ mixture the lifetime of the roton branch of the system plasmon-roton mode is comparable or even shorter than the mode period, i.e., that this branch is virtual or strongly decaying. In the ternary mixture $D^+$-$T^+$-$^3He^{++}$ this branch's decrement is found to be smaller than its frequency, so that it becomes observable. The form of the calculated dynamic structure factors confirms these results. Conditions are established for the mixture dielectric function to lose its analyticity in the complex frequency upper half-plane [4, 5], and the relative

contributions to the *f* -sum rule of the unique pole located on the positive part of the imaginary axis called the “ghost plasmon” and of other two poles located in the lower half-plane are found. In Fig. circles and diamonds stand for the real and imaginary parts of the plasmon-roton mode, and squares correspond to the imaginary parts of the dielectric function pole on the complex frequency upper half-plane.

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# Ion Temperature Measurements in Dense Compressed Solids

Michael Larsen[1], Thomas White[1], Travis Griffin[1], Daniel Haden[1], Hae Ja Lee[2], Eric Galtier[2], Eric Cunningham[2], Dimitri Khaghani[2], Lennard Wollenweber[3], Ben Armentrout[2], Carson Convery[2], Karen Appel[3], Luke Fletcher[2], Sebastian Goede[3], Jerome Hastings[2], Jeremy Iratcabal[1], Emma McBride[4], Jacob Molina[1, 5], Giulio Monaco[6], Landon Morrison[1, 7], Hunter Stramel[1], Sameen Yunus[2, 8], Ulf Zastrau[3], Siegfried Glenzer[2], Gianluca Gregori[7], Dirk Gericke[9], Bob Nagler[2]

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Advancing our understanding of material behavior under extreme conditions is crucial for breakthroughs in geophysics, astrophysics, and shock physics. Central to this pursuit is the precise measurement of the equation of state (EOS), delineating how materials react to changes in temperature, pressure, and density. Yet the accurate determination of temperature - a pivotal element of EOS - poses significant challenges, especially in dense, opaque materials prevalent in dynamic compression studies. To address this gap, we have pioneered an approach utilizing high-resolution X-ray scattering technology at free-electron laser facilities. The inelastic X-ray scattering at millielectronvolt energies (meV-IXS) platform leverages a monochromatic X-ray source to penetrate dense matter, allowing us to measure the ion temperature. In backscattering geometry at high temperatures, we observe Doppler broadening of the Rayleigh peak, providing a model-independent assessment of temperature through the ion velocity distribution. However, for highly compressed solids that remain below the melt temperature, the presence of phonons complicates the analysis. In this work, we use multi-phonon calculations and molecular dynamic simulations to investigate how X-ray scattering spectra relate to ion temperature for solid matter.

# Design of a Thomson parabola ion spectrometer for high-intensity short-pulse laser experiments at MEC

Andrea Zabala[1]

[1]SLAC National Accelerator Laboratory

In high-intensity laser-plasma interactions, characterizing ion species and their energy distributions is crucial for monitoring laser-matter interaction and understanding fundamental processes at the origin of laser acceleration of charged particles. At the Matter in Extreme Conditions (MEC) instrument of the Linac Coherent Light Source (LCLS), we are developing a Thomson Parabola Ion Spectrometer (TPS) specifically tailored for use with the short-pulse laser configuration. This diagnostic tool will allow for charge-resolved ion detection by utilizing combined electric and magnetic fields to deflect charged particles according to their charge-to-mass ratios and kinetic energy. The TPS is being designed for use in the MEC target chamber while taking into consideration the constraints of the optical laser and chamber dimensions. It will feature custom made micro-channel plate (MCP) stacks, boasting significant advantages, such as compatibility with high repetition rates and electromagnetic pulse (EMP) conditions. It will serve as a valuable tool for laser-plasma experiments, capable of measuring a wide range of accelerated ions. Current research is focused on calculating magnetic field guidelines to later perform trajectory simulations that will optimize the TPS design for implementation in upcoming experiments. This will enable more in-depth investigation of parameters such as maximum ion energy under varying laser conditions and target materials. This project not only improves MEC's experimental capabilities but also provides a hands-on opportunity to apply principles of electromagnetism, charged particle optics, and detector physics in a high-impact research environment.

# Utilizing Stochastic Correlation Spectroscopy for High Resolution X-Ray Scattering from Warm Dense Matter

Lex Andersen[1], Luke Fletcher[1], Willow Martin[1, 2], Siegfried Glenzer[1], Jerry Hastings[1], Madison Singleton[1], Emma McBride[3], Adrien Descamps[3], Sebastian Goede[4], Ulf Zastrau[4], Peihao Sun[5], Iris Kunz[1]

[1]SLAC National Accelerator Laboratory, [2]Physics Department, Stanford University, [3]Queen's University of Belfast, [4]European XFEL, [5]University of Padova

Warm Dense Matter (WDM) presents a unique challenge for theoretical modelling due to both ion-ion interactions and partially degenerate electrons being present. As current condensed

matter theory and plasma physics theory are inadequate for predicting WDM conditions, implementing high resolution stochastic correlation x-ray spectroscopy will provide accurate measurements of electron temperature and average ionization with an improved signal-to-noise ratio. This diagnostic uses the correlation of individual incident, non-monochromatized SASE pulses and the corresponding X-ray Thomson scattering (XRTS) to reconstruct the full dynamic structure factor. Requiring an accurate measurement of the incoming free electron laser, we construct a single shot hard X-ray spectrometer with a flat silicone crystal which yields results that are spatially and spectrally uniform. Initially measuring the collective forward scattering of cold aluminum at European XFEL, we demonstrate eV-scale resolution, benchmarking our results with multi-component scattering simulations (MCSS). Stochastic Correlation Spectroscopy is being fielded at SACLA, taking advantage of the two color modes to pump and probe at two unique photon energies. By analyzing isochorically heated copper and nickel in the WDM regime, we hope to provide accurate plasma parameters and low signal-to-noise XRTS to constrain plasma modelling parameters.

## On-the-fly machine learning studies of nickel in Mars core conditions

Maitrayee Ghosh[1], Arianna Gleason-Holbrook[1], Siegfried Glenzer[1]

[1]SLAC National Accelerator Laboratory

The warm dense matter (WDM) conditions - characterized by gigapascal pressures and few thousands of Kelvin temperature, are observed in the planetary interiors. Besides experimental techniques, atomistic simulations, particularly based on density-functional theory (DFT), play a key role in elucidating the microscopic properties in the WDM regime. However, accurate DFT-molecular dynamics (MD) suffer from major limitations of small cell sizes (up to 500-1000 atoms), few picoseconds of simulation, and high computational cost.

In this presentation, we demonstrate the use of density-functional theory coupled with on-the-fly machine learning strategy, as implemented in the Vienna *ab initio* Simulation Package (VASP) [1, 2], to overcome the finite size limitations of DFT. This approach dynamically trains a machine-learned force field (MLFF) during the simulation, allowing the model to bypass computationally expensive DFT calculations when sufficient accuracy has been achieved, thereby accelerating the overall computation [3].

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# Measurement of interfacial thermal resistance in high-energy-density matter

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Heat transport throughout high-energy-density systems and across interfaces is a ubiquitous phenomenon with many unresolved aspects. In particular, thermal conductivity in warm dense matter has extensive theoretical predictions but lacks experimental benchmarking [1]. We use Fresnel diffractive radiography [2-4] to measure the interface evolution in an isochorically-heated plastic-coated tungsten wire. After pressure equilibration, the interface is hydrodynamically stable and its evolution is driven primarily through thermal conduction, which modifies the temperature and density profiles. We find experimental evidence of a significant and long-lasting thermal barrier between the warm dense tungsten and its surrounding plastic. This temperature jump is characteristically similar to temperature jumps resulting from interfacial thermal resistance [5], indicating that the phenomenon can play a significant role in these extreme conditions, despite an abundance of free electrons [6]. The restricted heat flow may be of particular importance for inertial confinement fusion experiments, where instability-prone material interfaces play a large role in determining capsule implosion performance [7].

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# Modeling the Sn Equation of State to Constrain the Liquid Vapor Dome

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The off-Hugoniot expanded states of matter remain poorly understood for several materials of interest to the national defense and planetary impact communities. Predictive modeling of phase

transformations remains limited—specifically in the onset of vaporization in Sn under high-pressure conditions. To address this gap, we have developed an equation of state (EOS) model using the analytical modeling software ANEOS, which uses current expanded states data to predict the location of the liquid-vapor equilibrium region. This has allowed for a more comprehensive understanding of the thermodynamic behavior of Sn. Our equation of state has also enabled us to investigate Sn response to impacts with different materials in the 2D hydrocode simulation software, PyKO. Our model will help to inform the design of future planar impact experiments on our single stage and two stage light gas guns in order to best constrain the Sn equation of state.

## Estimates of the dynamic structure factor for the finite temperature electron liquid via analytic continuation of path integral Monte Carlo data

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Path integral Monte Carlo (PIMC) simulations are one of the few methods which can describe the structure of the plasma in Warm Dense Matter. However, the imaginary time correlation functions (ITCF) estimated by PIMC simulations must be analytically continuated back to real time to extract dynamic information about the system. One of the most ubiquitous approaches to analytic continuation is the maximum entropy method (MEM). The MEM is typically used with Bryan's controversial algorithm [Rothkopf, "Bryan's Maximum Entropy Method" Data 5.3 (2020)]. We investigate a dual Newton optimization algorithm to be used within the MEM that addresses known issues. We pay special attention to our uncertainty providing analytic bounds for the algorithm's error as well as numerical estimates of the uncertainty arising from both the ITCF and the regularization weight. We use the MEM to investigate authentic PIMC data for the uniform electron gas and further substantiate the roton-type feature in the dispersion relation. This work demonstrates that the all-purpose maximum entropy method can reliably estimate the DSF from PIMC data and establishes a path towards model-free estimates of the DSF in ion-electron systems.

## Roadmap to frequency dependent opacities from DFT-MD simulations

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The frequency-dependent opacities of materials under extreme conditions play a central role in the interpretation of astrophysical observations and the design of high-energy-density experiments. In this work, we compute the dielectric function and resulting opacities of warm dense hydrogen using density function theory but also time-dependent density functional theory. We combine low-frequency intraband contributions—relevant for transport properties—with high-energy interband transitions, which dominate XUV and soft X-ray absorption. This two-step approach enables a consistent treatment of both metallic and bound-electron effects across a wide frequency range.

## Predicting the uniform electron gas stopping power at moderate and strong coupling

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We present a detailed study of the stopping power of a homogeneous electron gas in moderate and strong coupling regimes using the self-consistent version of the method of moments [1-5] as the key theoretical approach capable of expressing the dynamic characteristics of the system in terms of the static ones, which are the moments. We develop a robust framework, which relies on nine sum rules and other exact relationships to analyze electron-electron interactions and their impact on energy loss processes. We derive an expression for the polarizational stopping power that takes into account both quantum statistical and electron correlation effects. Our results demonstrate significant deviations from classical stopping power predictions [6-8] (see Fig.), especially under the strong coupling regime, when electron dynamics is highly dependent on the collective behavior presenting two collective modes, each of them interacting with the incoming projectile separately. This work not only advances the theoretical understanding of the uniform electron fluid but also has implications for practical applications in fields such as plasma physics and materials science.

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*Acknowledgements. This research was supported by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan under Grant #AP09260349 and Ministry of Science and Innovation, Spain, under Grant #PID2021-127381NB-I00.*

# Inverse Supersymmetry in Finite Temperature Bose-Fermi Mixtures

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We investigate near-supersymmetric Bose-Fermi mixtures at temperatures greater than the condensation temperature of the constituent bosons. In this regime, we describe the breaking of supersymmetry (SUSY) between bosons and fermions with up to two internal states through the emergence of fermionic Goldstino modes. We draw a distinction between typical SUSY, where bosons have pseudospin 0 and fermions have pseudospin 1/2, and inverse supersymmetry (iSUSY), where bosons have pseudospin 1/2 and fermions have pseudospin 0. We highlight that the Goldstino pseudospin is carried by either its constituent fermion (SUSY) or boson (iSUSY). We then distinguish between these two cases by depicting their differing effects on the spectral function of the fermionic atomic species. Lastly, we propose an RF-spectroscopy measurement, analogous to momentum (angular) resolved photoemission in condensed matter physics, to measure the pseudospin-dependent spectral function.

# Ionization and Partition Function Regularization in Multicomponent Warm Dense Matter

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The study of warm dense matter (WDM) is crucial for understanding extreme physical environments, such as the interiors of astrophysical objects, nuclear explosions, and inertial confinement fusion experiments. It is known that WDM exhibits unique properties distinct from both classical gases and condensed matter, making it a key focus of both fundamental and applied research. A major challenge in this field is the development of accurate theoretical models capable of describing matter under such extreme conditions.

Computational modeling plays a vital role in WDM research, bridging gaps in experimental data. In contrast. this study employs a generalized chemical model for multicomponent systems that allows for the derivation of analytical expressions for the composition and thermodynamic properties of the medium. A key advantage of this model is its flexibility in incorporating an arbitrary number of components and any type of interaction potentials in the Helmholtz free energy, and thereby enabling unified treatment of diverse problems.

A significant issue addressed herein is the divergence of the internal partition function for composite particles in the ideal gas approximation. In our approach, each excited state is treated as a distinct species with a single energy level. The inclusion of interparticle interactions enables the identification of critical quantum numbers beyond which level populations vanish.

Unlike traditional methods of truncating the partition function, the proposed approach naturally excludes states whose excitation energies exceed the ionization potential lowering (IPL). These states are no longer physically relevant as they transition into the continuum. The IPL from excited levels is calculated by minimizing the total Helmholtz free energy, allowing the determination of the threshold at which excited states become delocalized.

# Theoretical perspectives on the stability and phase transitions of $MgO_2$ at Earth's mantle conditions

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Magnesium and oxygen are two of the most abundant elements in terrestrial planets, and their compounds—especially MgO—form the foundation of planetary mantle models. However, the high oxygen fugacity in planetary mantles can possibly form superoxides that have O stoichiometries higher than MgO. Understanding the extreme condition behavior of these Mg-superoxides can thus improve our understanding of their composition, seismic behavior, and thermal evolution of the oxygen-rich mantles of Earth-like exoplanets.

The present work specifically focuses on understanding the high pressure and high temperature behavior of $MgO_2$. Although thermodynamically unstable at ambient conditions, past crystal structure searches performed at 0 K has indicated that $MgO_2$ can be stable above 116 GPa till ~600 GPa [1]. Further, static compression experiments using diamond anvil cells have indicated that $MgO_2$ can become thermodynamically stable at pressures above ~96 GPa till 2150 K [2].

In the present study, we investigate the temperature-dependent dynamical stability of $MgO_2$ at ~100 GPa using first-principles phonon calculations within the quasi-harmonic approximation coupled with the anharmonicity from the density-functional theory (*DFT*) based molecular dynamics (*MD*) simulations. We analyze the phonon dispersion relations of different solid phases of $MgO_2$ across a wide pressure-temperature range to identify regions where the structure remains dynamically stable. Using the *DFT-MD* simulations, we further extend our understanding of possible phase transitions including melting of $MgO_2$ in our *P-T* conditions of interest. We expect the present results on the high-pressure phase stability of $MgO_2$ can have important impacts in high energy density sciences and planetary sciences.

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# Thermal Conductivity and Shock Ringing in Warm Dense Matter

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The performance of inertial confinement fusion (ICF) implosions is highly dependent on the transport properties of the materials involved, but experimental data for these properties remains sparse. This is largely due to the inherent difficulty in probing matter at high energy densities (HED), and has lead to a reliance on numerical modelling to quantify material properties at these conditions. However, predictions of transport properties are not well constrained, with order-of-magnitude variations between models even for well-studied materials at the same densities and temperatures. Here we present our latest progress in developing a method to infer the thermal conductivity of ablator materials in multi-layer targets irradiated by a high-energy laser. In such geometries, reverberating compression waves arise from the impedance gradients at material boundaries; using a Spitzer-Hãrm conduction model, we find that the amplitude and length scale of these waves are strongly coupled to material thermal conductivities. This opens up the possibility of constraining simulated conductivities in ICF-relevant materials at HED conditions by using x-ray imaging to measure shock ringing experimentally. We present preliminary results for Kapton using data from void collapse experiments at the Linac Coherent Light Source (LCLS), and find conductivities that are within an order of magnitude of existing models.

# Diffusion Coefficients of Warm Dense Water

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We investigate the phase-dependent diffusion behavior of water under extreme conditions using first-principles molecular dynamics simulations. Mean square displacements are analyzed to extract diffusion coefficients for hydrogen and oxygen in the liquid, solid, and superionic regimes. The results provide insight into ionic mobility across phase boundaries and are relevant for

understanding water-rich planetary interiors. Particular emphasis is placed on identifying the onset of superionicity and the suppression of diffusion in the solid state.

## Advancing diagnostic capabilities for warm-dense matter on the National Ignition Facility

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X-ray scattering is a powerful diagnostic for characterizing warm-dense matter, as it simultaneously encodes details of electron correlations, ionization, and the plasma thermodynamic state [S. H. Glenzer and R. Redmer, Rev. Mod. Phys. 81, 1625 (2009).] However, scattering measurements from laser-driven samples must contend with not only a short-lived and rapidly evolving state but also weak scattering cross-sections. A continuous scattering measurement would provide unprecedented access to the ion-plasma interaction while also characterizing the evolving thermodynamic state. To provide the required diagnostic capability, we have designed a high-efficiency x-ray spectrometer coupled to a streak camera for use on the National Ignition Facility. The spectrometer utilizes a conically curved crystal to increase solid angle collection and to sagitally focus the signal onto the 1-mm wide streak camera slit. The resulting continuous record enables reconstruction of the full experiment history from a single experiment, not only increasing data collection per experiment by a factor of five relative to existing spectrometers [T. Döppner, et al., Rev. Sci. Instrum. 85 (2014)] but also eliminating the uncertainty introduced by combining data from multiple shots. Two applications will be discussed: improved constraint of pressure-induced electron delocalization in implosions [T. Döppner, et al., Nature 618, 270 (2023)] and temperature diagnosis of doubly-shocked foams [M. J. MacDonald, et al., Phys. Plasmas 30 (2023)].

This work was performed under the auspices of the U.S. Department of Energy and an appointment to the Office of Science, by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

## A new Gross-Pitaevskii approach for exciton superfluids and incompressible supersolids

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Reports of condensation [1,2] of dipolar excitons have drawn much attention to excitonic bilayer semiconductor systems in which electrons and holes are confined in separate layers. In a variational calculation, we have predicted a transition to an incompressible supersolid with one exciton per site [3].

We investigate the superfluid and supersolid ground states with a time-dependent Gross-Pitaevskii approach for the dipolar excitonic system. Here the interaction between excitons is purely repulsive dipole-dipole, in contrast with ultracold dipolar gases [4], where the effective interaction contains attractive and repulsive parts. We construct a new Gross-Pitaevskii formalism to exclude the self-interaction of excitons on single occupancy sites, and to take into account two-particle correlations. The T=0 Gross-Pitaevskii admits both superfluid and incompressible supersolid ground state solutions dependent on layer separation and exciton density.

We further investigate the formation of vortices in the exciton superfluid, since observation of vortices is generally used to establish the existence of condensation [5] and to characterize a superfluid to supersolid transition [6].

We describe the properties, interactions, and lattices of the vortices while tuning the layer separation and density. An interesting picture emerges since a density pileup and saturation of the vortex radius occur at the superfluid-to-supersolid transition. At the transition, the vortices are compact to fully fit within unit cells of the incompressible supersolid.


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# The finite temperature 2D UEG: dielectric schemes and ab initio path integral Monte Carlo simulations


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There have been numerous advances in the description of the finite temperature 3D uniform electron gas (UEG) both in quantum Monte Carlo simulations [1,2] and in the self-consistent dielectric formalism [3,4,5]. Unfortunately, 2D UEG investigations have been limited to the ground state limit [6] with a near-absence of reliable results for the finite temperature 2D UEG [7]. Nevertheless, advances in semiconductor applications will likely require taking into account the electronic temperature in the future. We present extensive thermodynamic and structural results

for the finite temperature 2D UEG within the self-consistent dielectric formalism. In particular, 2D versions of the Singwi-Tosi-Land-Sjölander (STLS) scheme that is tailor made for weak-to-moderate coupling [8] and the hypernetted-chain (HNC) scheme that is tailor made for moderate-to-strong coupling [9] have been developed. Efficient numerical schemes have been devised for their accurate solution; the 2D-STLS scheme benefits from the emergence of complete elliptic integrals of the first and second kind, while the 2D-HNC scheme benefits from the use of the bipolar convolution theorem. A detailed comparison with new Path Integral Monte Carlo results is carried out.

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# Dense and Astrophysical Plasmas Session 2

## The outer planets and the H-He-C-O system

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The outer planets are of interdisciplinary interest. They serve as giant laboratories for studying the lightest and most abundant elements in the universe (H,He,O,C), although stable layers can prevent a direct probing of equations of state. Giant planets carry the composition of the early solar system, although subsequent mixing, demixing, and atmospheric pollution can make direct composition inferrence  pretty hard. In the ice giants, C can form diamonds, while the gas giants harbor conditions where C is predicted to adopt the BC8 phase. These materials are of high technological interest.

Jupiter's atmospheric temperature suggests that the interior is cool, less than 5000 K, in the 10-100 GPa region;  under those P-T conditions, DFT-MD method based H-He EOS predict rather high densities.  A low density on the other hand is indicated by the gravity data from NASA's Juno mission. Apparently, there is a density-tension problem. I will inform about the different proposed solutions. They all rely on the occurrence of H/He phase separation in the Mbar region. There is a clear gap between evidence of H/He phase separation from observations and modeling as well as simulations, and the indication thereof from unconfirmed experimental results.

The opposite holds for Uranus, Neptune, and the H-C-O system: phase separation is investigated both experimentally and using simulations, while interior and evolution models have just begun to apply those data. First results are surprising:  1, the common and otherwise unexplained

three-layer structure assumption can be the result of H2/H2O phase separation; 2. the structural adjustment against gravity requires an additional energy source: diamond rain?

A possible ice giant interior structure which is informed by current knowledge of the H-C-O system is illustrated in the Figure.

## Free-Free Absorption in Dense Hydrogen Plasmas Relevant to Stellar Interiors

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Opacity plays a critical role in determining energy transport within stellar interiors, directly influencing the boundary between radiative and convective zones. However, the opacity of hydrogen under stellar core conditions remains poorly constrained, both experimentally and theoretically. Modeling such environments is challenging due to the extreme plasma conditions involved—temperatures of several hundred electronvolts and densities hundreds of times greater than solid matter—which are difficult to replicate and compute accurately.

We report the first measurements of hydrogen absorption under conditions relevant to stellar interiors, conducted at the National Ignition Facility. To interpret the data, we employ a modeling approach that avoids the need for costly hydrodynamic simulations, enabling more tractable analysis. Furthermore, our methodology incorporates Bayesian inference to rigorously quantify uncertainties in the inferred opacity. These results provide key experimental benchmarks for hydrogen opacity in high-energy-density plasmas and will offer new insights into energy transport processes in stellar environments.

## A conductivity model for hydrogen based on ab initio simulations

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Models for the electrical and thermal conductivity of dense plasmas have been developed, e.g., by Lee and More [1] based on the relaxation time approximation for the Boltzmann equation and by Ichimaru and Tanaka [2] using a quantum statistical approach for the evaluation of the Ziman formula. We calculate the electrical and thermal conductivity of hydrogen for a wide range of

densities and temperatures by using molecular dynamics simulations informed by density functional theory [3]. Based on the corresponding extended ab initio data set, we construct interpolation formulae covering the range from low-density, high-temperature to high-density, low-temperature plasmas. Our conductivity model reproduces the well-known limits of the Spitzer and Ziman theory. We compare with available experimental data and find very good agreement. The new conductivity model can be applied, e.g., in dynamo simulations for the magnetic field generation in gas giant planets, Brown Dwarfs, and stellar envelopes.

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## Spectroscopic studies of hot dense plasmas isochorically heated by XFEL

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The characteristics of solid-density plasma in the hot dense matter regime is crucial for the study of stellar matter and inertial confinement fusion. However, many phenomena, such as nonlinear transport, partial ionization, strong coupling, and atomic processes, are poorly understood under such conditions. With the advent of the X-ray free-electron lasers (XFEL), intense x-ray radiation, in excess of $10^{17}$ W/cm$^2$ at hard X-ray photon energies, can be applied to samples to create and probe such hot dense plasma under well-defined conditions. We applied intense XFEL beam to 2 or 10 micron thick metal foils and observed emissions during transitions from L or M shells to the K shell. Satellite K-alpha emissions will be compared with CCFLY calculations and discussed for different charge states and Z.

# Dense and Astrophysical Plasmas Session 3

## Towards holistic approaches for the interpretation of X-ray Thomson Scattering experiments

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Understanding the microscopic states present in dense plasmas is one of the grand challenges in high-energy density physics. This is particularly true in the warm dense matter regime, characterized by a complex interplay of long-range Coulomb interactions, quantum many-body effects, and thermal energies on the order of several eVs. Theoretical models in this regime require careful inspection, as many are constructed based on ground-state theories or

low-temperature assumptions and may not adequately describe plasma behavior under these conditions. While spectroscopic data or absorption measurements can deliver valuable insights, they require preliminary model information about the atomic physics in this regime that are currently not well understood. X-ray Thomson Scattering (XRTS) differs from this as a diagnostic technique as the observable it probes is the density-density correlation function at finite temperature. To fully understand the microscopic physics of dense plasmas, one must carefully evaluate the validity of approximate XRTS theories in these regimes and compare them to full *ab initio* simulations. In this presentation, we give an overview of recent advances on the theory behind XRTS from imaginary-time correlation functions (ITCF) and how to appropriately quantify model uncertainties using established Bayesian inference techniques. Additionally, we present the most recent advances from path-integral Monte Carlo simulations as an exact *ab initio* simulation technique to compare against results from experiments and density functional theory simulations. This is furthermore accompanied by showing how recently developed ray-tracing capabilities enable a promising way to achieve comprehensive simulations of XRTS experiments.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 and supported by Laboratory Directed Research and Development (LDRD) Grants No. 25-ERD-047.

# Non-Equilibrium Systems Session 2

## Quantum Fluctuations Approach to Strongly Coupled Coulomb Systems Out of Equilibrium

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The theoretical description of strongly coupled quantum many-body systems out of equilibrium is a significant challenge across many areas, including condensed matter, dense plasmas, and ultracold atoms. Standard approaches used for the description of the dynamics of such systems include the formalisms of reduced density matrices (RDM) and nonequilibrium Green's functions (NEGF). However, all approaches suited for the description of nonequilibrium quantum systems are limited in their applicability due to their accuracy or their unfavorable numerical scaling with respect to system size or propagation time. It is, therefore, important to develop new methods that strike a suitable balance between accuracy and computational complexity. Here, we present an alternative approach for describing the dynamics of quantum systems based on fluctuations of field operator products and their correlation functions [1,2]. Quantum fluctuations are closely related to NEGF and RDM theory and offer an alternative approach to the description of strongly coupled systems while exhibiting interesting complementary features, such as the capability to simulate many-body effects using stochastic methods [3,4]. This significantly reduces numerical complexity while maintaining accuracy and improving numerical stability compared to standard NEGF and RDM approaches.

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## Ultrafast Charge Separation on the Nanoscale Induced by a Uniform Field

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When illuminated by white light, atoms, molecules, and materials absorb only certain characteristic energy contributions based on their absorption properties. Here, we show that this effect can be translated from energy to space: a spatially uniform laser pulse can create strongly localized carrier excitations and spatial charge separation on the sub-nanometer scale within a few femtoseconds, possibly opening new avenues for nanoelectronics [1]. A promising candidate are small graphene heterostructures, which exhibit a pronounced space dependence of the DOS with strongly localized topologically protected states [2]. Direct evidence for this effect is presented by performing extensive NEGF simulations for these systems that take into account strong coupling and dynamical screening [3,4,5]. We demonstrate multiple ways to excite targeted areas of the nanostructures, such as a proper choice of the laser energy, polarization, or carrier-envelope phase. Moreover, we find that the observed effects strongly depend on the effective Coulomb interaction. While the targeted charge excitation greatly benefits from surface screening, in free-standing systems it is severely restricted by strongly bound excitons. The findings are expected to be applicable for a broad class of nanoscale monolayer clusters of graphene or TMDCs.

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# Others

## Configurational entropy of strongly coupled 2D finite clusters in dusty plasma

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Shell structures and configurational transitions in two-dimensional (2D) Coulomb systems have been extensively investigated within condensed matter physics [1]. Due to their quantum scales, pure Coulomb crystals are extremely fragile to produce experimentally and are generally studied via numerical simulations and models. However, in dusty (complex) plasmas, charged dust particles interacting with screened-Coulomb potential, can be of micro-meter size, enabling direct and accurate measurement of individual particle positions and velocities. We introduce a novel mechanical assembly, BECAA (Bidirectional Electrode Control Arm Assembly [2]), which enables the rapid formation of perfect 2D finite N-Clusters, where N can be precisely set from a single particle to large numbers within minutes, all while maintaining constant background discharge conditions. Using BECAA, we generate strongly coupled N-Clusters (N=1-30) and perturb their crystalline shell structures with multiple heating and cooling cycles (shown in Figure for cluster N=19) using randomized high-power laser beams to statistically identify both ground and metastable states and extract configurational entropy [3] based on the occurrence probabilities of each state.

Supporting grants: US Department of Energy (DOE) FY2020 Early Career Award DE-SC0021106 and Facilities Award DE-SC0023416.

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# Interaction of Hydrogen and Deuterium Cluster Ions with H2/D2 Gas and ZrDx Targets

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Fusion reactions in the core of sun and laser inertial confinement fusion (ICF) occur in extreme high dense plasma environments. Thus, understanding multi-body collisions in dense plasmas is essential for interpreting the micro-mechanism of fusion in Sun and ICF. In this work, the interaction of hydrogen and deuterium cluster ions ($H_n^+/D_n^+$, n=1,2,3) with hydrogen and deuterium gas ($H_2/D_2$) target and the $D(d,p)^3He$ fusion reaction induced by $D_n^+$ on $ZrD_x$ target are studied. The $H_n^+/D_n^+$ and $H_2/D_2$ collision experiment have been conducted at the electron cyclotron resonance ion source (ECRIS) in the institute of nuclear research, Debrecen, Hungary. $H_n^+/D_n^+$ ions with 4-10 keV/H(D) were used as projectiles to bombard $H_2/D_2$ jet target. A field-free time-of-flight (FFTOF) setup was used to measure the angular and energy distribution of recoils.

The results demonstrate the cluster effects are present in gas phase, but different by using $H_n^+$ and $D_n^+$ as projectile. The D-D fusion experiment was conducted at the duo-beam experimental chamber in the laboratory of accelerator and radiation technology, University of Lisbon. $D_2^+$ and $D_3^+$ ions in the energy between 20 keV/D and 26 keV/D from the 210KV ion implanter were used to bombard $ZrD_x$ target and protons emitted from $D(p,t)^3He$ reaction were detected by a SSD detector. $^3He$ ion beam with 1.25MeV from the 2.5MV Van de Graaf accelerator was used for measuring the deuterium concentration and distribution in $ZrD_x$ target before and after each D-D reaction measurement. Preliminary results show that, the proton yields induced by $D_2^+$ and $D_3^+$ ions are evidently different at the equivalent energy per-nucleon. It implies the fusion in multi-body collision environment might be different from simple binary nuclei fusion. Further study with deuteron(d) beam and in lower energy region should be conducted in future.

## Interaction of hydrogen and deuterium cluster ions with H2/D2 gas and solids

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Need to be filled later

## Ion and Electron Temperatures in 1-MA-Driven X-Pinch Plasmas via High-Resolution Ti Heβ Line Shapes

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X-ray emission spectra are rich in information about source plasma conditions, especially from high-density plasmas where spectra are affected by Stark broadening. Stark broadened line shapes reflect an ensemble of shifts induced by plasma microfields, meaning that changes in plasma density, ion temperature, and electron temperature all induce changes in emitted line shapes [1]. We recently sought highly Stark broadened line shapes of Ti Heβ in an experimental campaign at ZEBRA, a 1-MA pulsed power facility capable of producing kJ of x-ray emission. By deploying X-pinch loads composed of Ti, we were able to produce strong signals of Ti Heβ with distinct line shapes which have not been seen before. The observed line shape shows several peaks: two are reminiscent of line shapes seen from laser-heated, solid-density emission and which vary in separation, signal-to-noise ratio, and intensity ratio from shot to shot [2, 3]. The relationship between these two peaks may yield information about relative ion versus electron

temperatures in X-pinch plasmas. A third peak is reminiscent of satellite emission but is not consistent with previously observed satellite wavelengths; one hypothesis is that this peak may be a highly Stark-broadened component of Ti Heβ, or emission related to a high-density X-pinch phase where plasmas are tightly compressed by magnetic fields. We will present an initial analysis of measured line shapes, challenges in interpretation from time integration, and possible implications for X-pinch dynamics and electron-ion equilibration in hot-dense plasmas.

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# Dynamic compression of water at ice giant conditions

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Water exhibits one of the most complex phase diagrams, with over 19 distinct crystalline structures [1]. Among these, superionic ice has attracted attention for its unique property: a rigid lattice of oxygen atoms through which hydrogen diffuses rapidly. This exotic state of matter is believed to exist in the interiors of icy giant planets such as Uranus and Neptune, where extreme P-T conditions prevail. Early theoretical studies proposed a uniform superionic phase with a BCC oxygen lattice, inherited from ice VII or X [2,3]. However, later calculations suggested that an FCC lattice is thermodynamically favored, potentially impacting proton diffusivity [4]. As a result, numerous experimental efforts have aimed to map the stability domains and melting curves of these two superionic phases. Yet, findings often diverge at both low (<1 Mbar) and high (>1 Mbar) pressures. At low P, results from diamond anvil cells are contradictory [5,6], while at higher P, data remain scarce due to the challenges of probing such conditions. Existing laser-driven shock compression results also remain inconsistent [7,8].

Here, we report on the phase diagram of pure water under extreme conditions, based on multiple shock compression experiments coupled with ultrafast X-ray diffraction. Our study spans pressures from 20 to 180 GPa and temperatures from 1000 to 3500 K. The quality of our diffraction patterns enables us to distinguish different oxygen sublattices in the superionic regime and challenge the purely FCC phase model previously proposed. At lower pressures, our results raise new questions about the mechanisms and kinetics of phase transitions. These findings offer new constraints on the stability field of superionic ices [5-8].

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# Surviving the Entropy Catastrophe: Redefining the Limit of Superheating

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The theoretical concept of the "entropy catastrophe" establishes a stability limit for superheated solids, predicting a maximum temperature of approximately three times the melting point before the crystalline phase becomes unstable [1]. In this work, we experimentally challenge this limit using ultra-fast heating and high-resolution inelastic X-ray scattering. Gold samples subjected to heating rates exceeding $10^{15}$ K/s reached temperatures over 14 times their melting point—far beyond the entropy catastrophe threshold—while maintaining their crystalline structure. This breakthrough was achieved by using a short-pulse optical laser to rapidly heat the material, followed by direct measurement of ion temperatures via high-resolution X-ray scattering with an X-ray free-electron laser. The rapid heating bypasses intermediate destabilizing events, known as the "hierarchy of catastrophes," and prevents lattice expansion, eliminating the expected thermodynamic instabilities [2,3]. Consequently, the solid-phase entropy remains below that of the liquid, suggesting a significantly higher—or potentially nonexistent—upper limit for superheating.

These findings fundamentally redefine the stability boundaries of matter under extreme conditions, with broad implications for laser-based materials processing, inertial confinement fusion, and the behavior of matter in planetary interiors. They underscore the critical role of ultrafast, nonequilibrium dynamics in extending the limits of phase stability far beyond conventional thermodynamic expectations. By enabling direct access to extreme superheated states, this work opens new experimental pathways for exploring exotic phases of matter previously considered inaccessible.

*Funding Acknowledgements*

This work was funded in part by the US DOE, NNSA (Award No. DE-NA0004039) and U.S. DOE, Office of Science, Office of Fusion Energy Science (Award No. DE-SC0019268).

# Experiments with shock waves in strong magnetic fields at the Zebra pulsed power generato

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The 1 MA Zebra pulsed power machine at UNR generates strong magnetic fields that can be used for many applications. We developed experiments to study shock waves in gaseous media in strong magnetic fields. Shock waves are generated by a 1ns laser pulse with energy of 10-20J focused into a gas jet in the field region of 1-2 MG. Diagnostics include vertical interferometry, shadowgraphy, and schlieren at wavelengths of 532 nm, and 266 nm and a 4-frame side on diagnostics. The results from laser diagnostics are presented, including visualization of shock waves, as well as the dynamics and structure of shock waves in the gas jet. A spread of the front along the magnetic field lines were observed. Some velocities of shock waves in hydrogen were >2000km/s. Generation of shock waves are simulated with a Helios and FLASH programs.

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