MSEE | MATERIALS SCIENCE IN EXTREME ENVIRONMENTS UNIVERSITY RESEARCH ALLIANCE

Seminar

Carbon at Extremes: Discovery Science with Exascale Computers and Experiment

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The behavior of carbon under extreme conditions pressures and temperatures is of key importance for understanding interiors of carbon-rich exoplanets and harnessing clean energy through inertial confinement fusion (ICF). The advent of powerful laser and pulsed-power compressions, in-situ X-ray synchrotron and free electron laser (XFEL) diffraction experiments provide unique opportunities to recreate and probe the high-PT environment of exoplanetary cores and ICF implosions in the laboratory. However, science return is limited due to difficulty of obtaining atomic-scale insight from these sophisticated and expensive experiments. By developing machine-learning models of interatomic interactions at extreme conditions and employing the most powerful computers in the world, we are able to simulate atomic-scale dynamics of materials response at experimental time and length scales in quantum accurate, billion atom molecular dynamics (MD) simulations. In this talk I will discuss several key insights including synthesis of long-sought BC8 high-pressure post-diamond phase of carbon, inelastic deformations in shocked diamond and complex phase transitions in carbon ICF ablator materials. These transformative simulations guide our experimental campaigns at NIF, Omega, and EuXFEL facilities towards observing predicted phenomena.

Ivan Oleynik is a professor at the Department of Physics, University of South Florida. His research focuses on studies of materials at extreme pressures and temperatures by advanced theory, simulations and experiment. He is also best known for design and prediction of properties of novel materials, and development of new methods for materials simulations at atomistic level. He leads several experimental teams to perform experiments at National Ignition Facility at Lawrence Livermore National Laboratory, Sandia's Z pulsed power facility, Omega laser facility at Laboratory of Laser Energetics to realize groundbreaking predictions from his simulations. He also spearheads several computational campaigns at DOE's exascale supercomputers, securing the largest computing allocations awarded by DOE's ASCR Leadership Class Computing Challenge (ALCC) and the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) programs. Ivan also led a team of computational scientists that earned a 2021 Gordon Bell Prize finalist nomination for record-breaking billion-atom simulations of carbon at extreme conditions and experimental time and length scales. He is a Fellow of the American Association for Advancement of Science, the American Physical Society, and the American Vacuum Society.

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