SACRAMENTO STATE

Department of Physics and Astronomy

SPRING 2023 Colloquium Series

"Quantum Simulations at Extreme Conditions: from Planetary Interiors to Dense Plasmas"

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Computer simulations based on quantum mechanics are useful because they are predictive. Approaches based on first-principles have demonstrated that the properties of matter can be predicted very accurately, even at extreme conditions of pressure and temperature present in shock or ramp compression experiments and planetary interiors [1,2]. Using these techniques, we can predict new phase transitions that occur at high pressure and obtain equations of state (EOS) of different materials, guiding state-of-the-art experiments that are able to achieve these conditions, and develop new theoretical models for matter at extreme conditions. I will show how quantum atomistic simulations, based density functional theory molecular dynamics (DFT-MD), can be used to study novel processes that occur at the interior of planets and exoplanets (outside our solar system) and constrain their interior structure, where the extreme conditions of pressure and temperature give rise to new chemistry and physics of materials. These calculations can guide shock compression experiments, where strong ionization of the atomic L-shell and K-shell [3,4] gives rise to warm dense matter (WDM) regime of dense plasmas. This progress in this field has enabled us to study the nonideal mixing effects in WDM [5] that we have used to generate new EOS of arbitrary mixtures of materials [6]. In addition, we show how DFT-MD simulations can be applied to address a number of problems relevant to planetary science, including the erosion of Jupiter's core [7], miscibility of planetary materials [8], and crystallization of super-Earth cores.

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4:00 – 5:20PM
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