Chemical and Biomolecular Engineering

Spring 2021 Seminar

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Physical and Life Sciences Directorate

Lawrence Livermore National Laboratory, Livermore, CA

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Achieving an Improved Understanding of Material Evolution Under Extreme Conditions with Artificial Intelligence

Abstract: Understanding evolution of organic molecular materials (OMMs) subject to extreme temperature and pressure conditions (e.g. 1000s of K and 10s of GPa) is crucial to fields spanning astrobiology to nanomaterial fabrication. However, a confluence of challenges leaves a clear picture of the governing phenomena elusive. Experimentally, these conditions are often realized by subjecting samples to shockwaves via detonation. Ensuing material evolution is rapid (e.g., occurring over nano-to-microsecond timescales) and often highly multiscaled, where reactivity, phase separation, and material strength are determined on approximately <100, 101, and 103 nm scales, respectively; as a result, direct experimental determination of many fundamental properties is intractable.

Atomistic simulations can be a powerful tool for shock experiment interpretation by both providing an atomistically-resolved view into OMM evolution and providing inputs (e.g. equation of state, chemical kinetics, etc.) necessary for larger-scale (e.g. continuum) models. However, characteristic problem scales approaching a μm and a μs preclude use of highly predictive first principles-based simulation approaches, and existing molecular mechanics-based interatomic models are generally not designed for such high temperature and pressure conditions.

In this seminar, an artificial intelligence-driven model development approach enabling "quantum-accurate" simulation at a fraction of the computational cost will be discussed. First-of-their-kind simulations that use resulting models will be presented, in which shockwave-induced chemistry in liquid carbon monoxide was found to yield nanocarbon condensates. Ultimately, these simulations have enabled resolution of decades old questions pertaining to the early mechanisms and kinetics governing detonation nanocarbon production.

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Bio: Dr. Rebecca Lindsey received her B.S. in Chemical Engineering from Wayne State University and her M.S. and Ph.D. in Chemical Physics from the University of Minnesota, Twin Cities. She was a postdoctoral researcher at Lawrence Livermore National Laboratory (LLNL), where she is currently a Staff Research Scientist. Her work in computational chemistry, for which applications have spanned sorption in soft materials, possible mechanisms for the origins of life, and detonation synthesis of unusual carbon nanoparticles, has been underpinned by a strong interest in developing tools enabling work in previously inaccessible problem spaces. Dr. Lindsey's efforts were recently recognized through a LLNL Physical and Life Sciences Directorate Research Award. In addition to her work in computational chemistry, she leverages data science and machine learning tools to aid in interpretation of large experimental datasets and to develop age-aware material performance models from them.