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Large Scale DFT Simulation of Materials under Extreme Conditions

Abstract: All materials can be accurately described by quantum mechanics (QM); however, even at a relatively simple level of approximation, size limitations have precluded QM from being applied toward complex heterogeneous systems of all material classes. Removal of the computational bottlenecks that restrict system sizes as well as inhibit treatment of unusual configurations allows heretofore unattainable quantum mechanical characterization of complex systems such as amorphous and disordered materials, interfaces, and doped and defected materials.

This talk will report recent efforts at the US Army Research Laboratory to employ large scale QM simulations to understand the atomistic behavior of a variety of materials under extreme conditions and the effects of disorder, interfaces, and defects have on these materials, as well as the shortfalls of the level of theory employed. The materials studied range the super-hard material Boron-Carbide, to the high energy explosive PETN.

Bio: William D. Mattson, Research Physicist, Weapons and Materials Research Directorate, U. S. Army Research Laboratory. Dr. Mattson obtained his B. S. in Physics and Computer Science at the University of Maryland Baltimore County in 1996, and his Ph.D. in Physics, University of Illinois at Urbana-Champaign, in 2003. He has worked for the Army Research Lab since 1993 and on his current work in the simulation of energetic materials since 1994. He developed and serves as the software development lead for the Institute for Multi-Scale Reactive Modeling of Insensitive Munitions, and the Quantum Mechanics for Material Science program at ARL. Dr. Mattson has also participated in developing scalable software for classical and quantum atomistic molecular and particle dynamics simulations and is currently working to extend the large scale density function theory calculations to hundreds of thousands of atoms and time steps for practical systems. Dr. Mattson currently serves as the Computational Technology Lead for Computational Chemistry, Physics, Material Science, and Biology for the DoD High Performance Computing Modernization Office.