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Density Functional Methods for Shock Physics and High Energy Density Science[1]

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Molecular dynamics with density functional theory has emerged over the last two decades as a powerful and accurate framework for calculating thermodynamic and transport properties with broad application to dynamic compression, high energy density science, and warm dense matter. These calculations have been extensively validated against shock and ramp wave experiments, are a principal component of high-fidelity equation of state generation, and are having wide-ranging impacts on inertial confinement fusion, planetary science, and shock physics research. In addition to thermodynamic properties, phase boundaries, and the equation of state, one also has access to electrical conductivity, thermal conductivity, and lower energy optical properties. Importantly, all these properties are obtained within the same theoretical framework and are manifestly consistent. In this talk I will give a brief history and overview of molecular dynamics with density functional theory and its use in calculating a wide variety of thermodynamic and transport properties for materials ranging from ambient to extreme conditions and with comparisons to experimental data. I will also discuss some of the limitations and difficulties, as well as active research areas.

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