Abstract Submitted
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**Accurate Density Functional Theory Simulations Across the Warm-Dense-Matter Regime: Thermal Meta-GGA Exchange Correlation and Nuclear Quantum Effects**[1] VALENTIN KARASIEV, DEYAN MIHAYLOV, SUXING HU, Laboratory for Laser Energetics, U. of Rochester — First-principles methods based on orbital-dependent and orbital-free density functional theory take into account the electron quantum effects and provide a compromise between reliability and computational efficiency for simulations of matter across extreme conditions of pressure and temperature in the warm-dense matter (WDM) regime. With that, the standard molecular dynamics approach treats ions classically within the Born–Oppenheimer approximation, omitting nuclear quantum effects (NQEs). The NQEs at high pressure are not negligible in a wide range of temperatures and must be taken into account for accurate predictions. In this talk we will discuss recent progress in the development of meta-generalized gradient approximation (meta-GGA) exchange- correlation functional enhanced by the GGA-level thermal corrections providing improved accuracy across the temperature regimes. Together with quantum treatment of ions via path integral molecular dynamics, our approach provides a systematically improved accuracy of WDM simulations, as we show in an example of dense hydrogen and deuterium plasmas.

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Valentin Karasiev
University of Rochester

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