Benchmarking consistent observable and material properties from an average-atom model to predictions from time-dependent density functional theory

Stephanie B Hansen¹, Thomas W Hentschel², Andrew D Baczewski¹, and Alina Kononov¹

¹Sandia National Laboratories
²Cornell University

Large-scale simulations of high energy density plasmas, such as those relevant to inertial confinement fusion and astrophysical objects, rely on knowledge of material properties across a wide range of temperatures and densities. Reliable simulations require both absolute accuracy in these material properties and internal consistency among them (e.g. they require that melt discontinuities in both conductivities and equations of state occur at the same conditions). Here, we describe an all-electron average-atom model based on density functional theory that calculates self-consistent electronic and ionic structure using spherically averaged potentials. These structures are used to predict internally consistent material and observable properties including equations of state, dynamic collisions and response, stopping powers, and x-ray emission, absorption, and scattering signatures on a wide range of temperature-density conditions. To test the accuracy of our average-atom model in warm dense matter conditions, where its imposed spherical symmetry is expected to falter, we compare its predictions to time-dependent density functional theory (TDDFT) models that have been extended to predict a variety of observable and material properties.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.