

Benchmarking pressures and ionization states for an average-atom model under warm dense matter conditions

Wednesday 14 September 2022 15:15 (30 minutes)

Average-atom models are an essential tool in modelling the warm dense matter regime, because they can be used to compute key quantities, such as equation-of-state data, for a fraction of the computational cost of higher-fidelity simulations such as DFT-MD. However, a variety of different models exist, and it is important to benchmark these models to understand their limitations and expected accuracy under various conditions. In this presentation, we focus on two key properties in WDM —the mean ionization state and pressure—for a range of materials, densities and temperatures. Through comparison with higher-fidelity simulations and experimental results, we probe the accuracy of an average-atom model, considering various choices of approximation within that model. We demonstrate a well-chosen average-atom model, under the right conditions, can yield close agreement with these benchmarks.

Primary author: CALLOW, Timothy (CASUS, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

Presenter: CALLOW, Timothy (CASUS, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

Session Classification: Afternoon Session (Wednesday)