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Resolving Warm Dense Aluminum with First-Principles and Machine-Learned MD Simulations

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Understanding warm dense matter relies on accurate theoretical input to interpret experimental observables such as X-ray Thomson scattering spectra. In this work, we perform density functional theory molecular dynamics simulations of aluminum to compute the static ion structure factor across a range of density-temperature conditions. To efficiently explore a finer grid, we train a neural network potential and run machine-learned molecular dynamics simulations. The resulting structure factors are used within a Bayesian inference framework to identify the most probable thermodynamic conditions realized in the experiment. Based on these conditions, we compute the electron dynamic structure factor using time-dependent density functional theory. This hybrid approach—combining ab initio simulations with machine learning and statistical inference—provides precise diagnostic support for interpreting scattering data and offers a robust framework for benchmarking theoretical models of warm dense matter.

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