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Ab initio simulations for the ion-ion structure factor of warm dense aluminum

Monday 21 February 2022 16:40 (30 minutes)

We present an extensive description of the application of a generalized collective modes model to ab initio simulations in the warm dense matter regime. We calculate the intermediate scattering function for warm dense aluminum by using density functional theory molecular dynamics simulations. From this data set we derive the static and dynamic ion-ion structure factors. Applying a generalized collective modes model, we can fit the excitation spectra of the ion system and thereby extract the dispersion for the ion acoustic modes, as well as the decay coefficients for the diffusive and collective modes. The results are discussed and compared with experimental data if available. We show that computational limitations prevent sufficient access to the hydrodynamic limit and demonstrate that this can be circumvented using machine learning.

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