

Abstract Submitted
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Bohm Molecular Dynamics Simulations of Warm Dense Matter¹

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KASIM, SAM VINKO, GIANLUCA GREGORI, University of Oxford — The com-
putational demands of modelling large numbers of coupled electrons and ions have
long been considered insurmountable, despite advances and refinements in density
functional theory (DFT) calculations. However, a different approach to modelling
quantum interactions, via application of the Bohmian trajectories formalism, can
overcome this hurdle. We present further results from a new Bohm - molecular
dynamics approach (Bohm MD). The static results of our simulations are validated
by DFT results – our static ion-ion structure factor of aluminium at 5.2 g cm^{-3}
and 3.5 eV shows excellent agreement with both orbital free and Kohn Sham DFT.
We then use Bohm MD to extract dynamic results, not only the ion-ion dynamic
structure factor which provides a direct link to experimental observables, but also,
unprecedentedly, the ion-electron and electron-electron dynamic structure factors.
Thus Bohm MD provides a self-consistent approach to non-adiabatic investigation
of dynamic modes in systems of thousands of particles.

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