Abstract Submitted
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Simple accurate first-principles pair potentials for studying linear transport properties of Warm Dense Matter[1] CHANDRE DHARMA-WARDANA[2], Retired — Density functional theory asserts that all the thermodynamic and linear transport properties are a functional of the one-body electron density $n(r)$ of an electron-ion system. If we consider a warm-dense matter (WDM) system it usually consists of an electron system and an ion system in equilibrium at some temperature T. We may consider any single representative ion in the WDM together with its neutralizing electron density distribution $n(r)$ around it as well as the ion distribution $\rho(r)$. The latter is the crystal structure if the system is a solid. In a fluid $\rho(r)$ is spherically symmetric and simple. Such a neutral object is known as a neutral pseudoatom. The $n(r)$ can be reconstructed to give the free electron pile up $\Delta n_f(r)$ at the ion in a uniform electron gas of the appropriate density. We have proposed (since the 1980s) the construction of simple linear local (i.e., s-wave) electron-ion potentials $U_{ei}(q)$ as well as second-order ion-ion pair potentials $V_{ij}(q)$ derived from $\Delta n_f(q)$ as an appropriate and usually accurate method for obtaining thermodynamic and transport properties of WDMs. We illustrate this approach by applications to Al, Li, C and Silicon WDM fluids as well as mixtures. [1]PHYSICAL REVIEW E 94, 053211 (2016)

[1]Nationa Research Council of Canada
[2]**Easy to construct accurate first principles pseuopotentials and pairpotentials for the study of linear transport properties of warm dense matter.**

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