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Pseudo-Atom Molecular Dynamics: A model for warm and hot dense matter[1]

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We have developed an efficient and versatile model to describe warm and hot dense matter that couples an average atom model with the integral fluid equations for the ion correlations. This model provides all bound and free electronic states and wave functions, the interaction potentials and all correlation functions without adjustable parameters. The electrons can be described quantum mechanically (Schrödinger equation) or semi-classically with the Thomas-Fermi model. The ion-ion pair potential can be used in a classical molecular dynamics simulation to yield equation of state and dynamic properties of dense plasmas, including mixtures. This "pseudo-atom molecular dynamics" model, or PAMD, is more approximate than ab initio methods such as Path Integral Monte Carlo and Density-Functional-Theory Molecular Dynamics but presents distinct computational advantages. Extensions of the model allow the calculation of diffusion coefficients, viscosity, X-ray Thomson Scattering spectra, DC conductivities and opacities. We will describe the model and present comparisons with ab initio simulations and experimental data in a wide range of applications. LA-UR-19-21380

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