

Abstract Submitted
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Pseudo-atom molecular dynamics for warm dense plasma mixtures CHARLES STARRETT, JEROME DALIGAULT, DIDIER SAUMON, Los Alamos National Laboratory — We have developed a new method for calculating the thermodynamics of warm dense mixtures. It combines an average atom-like approach to calculate the electronic structure of one “pseudo-atom” with classical molecular dynamics (MD) for the ionic structure. The result is a model in which both electronic and ionic structures of a plasma can be calculated rapidly and the resulting thermodynamics agree excellently with the much more expensive *ab initio* DFT-MD methods. We will present an outline of the new method and comparisons with DFT-MD for the ion-ion structure and the thermodynamics.

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