MAR09-2008-001582

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

Mixtures in the Warm, Dense Matter Regine[1]

LEE A. COLLINS, Los Alamos National Laboratory

The bulk of normal matter from planets to the intergalactic medium exists as a composite of various elemental constituents. The interactions among these different species determine the basic properties of such diverse environments. For dilute systems, simple gas laws serve well to describe the mixing. However, once the density and temperature increase, more sophisticated treatments of the electronic component and dynamics become necessary. For the warm, dense matter (WDM) region [10^{22}-10^{25} atoms/cm^3 and 300K - 10^6 K], quantum Monte Carlo and molecular dynamics, utilizing finite-temperature density functional theory (DFT), have served as the basic exploratory tools and benchmarks for other methods. The computational intensity of both methods, especially for mixtures, which require large sample sizes to attain statistical accuracy, has focused considerable attention on mixing prescriptions based on the properties of the pure atomic constituents. Though extensively utilized in many disciplines, these rules have received very little verification [1,2]. We examine the validity of two such rules, density and pressure mixing, for several systems and concentrations by comparing against quantum calculations for the fully-interacting composite. We find considerable differences in some regimes, especially for optical properties. We also probe dynamical properties such as diffusion and viscosity as well as the role of impurities. Finally, as a means of extending DFT results to higher temperature regimes, we also study orbital-free molecular dynamics (OFMD) approaches [3] based on various approximations to the basic density functional. These OFMD schemes permit a smooth transition from the WDM region to simpler one-component plasma and ideal gas models. Research in collaboration with J.D. Kress (LANL), D.A. Horner (LANL), and Flavien Lambert (CEA).

[1] D.A. Horner, J.D. Kress, and L.A. Collins, Phys. Rev. B **77**, 064102 (2008).
[2] F. Lambert *et. al.* Phys. Rev. E **77**, 026402 (2008); J. Clerouin *et. al.* Phys. Rev. B **76**, 064204 (2007).
[3] F. Lambert, J. Clerouin, and G. Zerah, Phys. Rev. E **73**, 016403 (2006).

[1]Work performed under the auspices of the U.S. Department of Energy.