Ab initio simulations for warm dense matter: phase transitions and isentropic shock compression experiments

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The behaviour of warm dense matter (pressures of several megabar and temperatures of several eV) is of paramount importance for interior models of giant planets such as Jupiter and Saturn. Strong correlations and quantum effects are important under those conditions which empede accurate predictions for the equation of state (EOS) and the high-pressure phase diagram of even the simplest and most abundant elements H and He. Furthermore, novel phenomena such as proton conduction and demixing are expected to occur in C, N, O, their hydrides, and mixtures at high pressures which are relevant for, e.g., Uranus and Neptune.

We apply ab initio molecular dynamics simulations based on finite-temperature density functional theory to calculate the EOS and the electrical conductivity for H, He, and their mixtures for a wide range of densities and temperatures. For instance, EOS data for hydrogen indicate a first-order liquid-liquid phase transition which is closely connected with a nonmetal-to-metal transition [1,2]. Our results yield a critical point at 1400 K, 1.32 Mbar and 0.79 g/cm^3 [2] – i.e. at much lower temperatures than chemical models have predicted for the plasma phase transition. Based on the ab initio EOS data we compare with available isentropic shock compression experiments [3-5]. The electrical and thermal conductivity, thermoelectric power, and Lorenz number are calculated [6]. We have identified the parameters for demixing of helium from hydrogen [7-9] which match the conditions in the interior of Saturn as long has been predicted.

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