DFT applied to warm dense matter

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The behavior of warm dense matter (pressures up to TPa and temperatures up to several eV) is of paramount importance for the interior, evolution and magnetic field of solar and extrasolar planets. While the light elements H and He are the main components of gas giants like Jupiter, mixtures of C-N-O-H are relevant for Neptune-like planets, and minerals of the MgO-FeO-SiO₂ complex are the building blocks of rocky planets (Earth, super-Earths). We apply molecular dynamics simulations based on finite-temperature DFT to calculate the equation of state, the high-pressure phase diagram, and the transport properties of warm dense matter for a wide range of densities and temperatures as typical for the interior of planets. Of special importance is the location of coexistence lines (melting) and possible demixing regions (H-He), and the treatment of nonmetal-to-metal transitions (metallization in H). We compare our results with shock-wave and x-ray scattering experiments and study their impact on planetary models. Challenges for DFT are the derivation of exchange-correlation functionals for finite temperatures, the correct prediction of band gaps, and the consideration of long-range (van der Waals) forces.