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Ab initio simulations for matter deep in the interior of giant planets: equation of state data and transport coefficients

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The behavior of warm dense matter (pressures of several Mbar and temperatures of several eV) is of paramount importance for interior and dynamo models of giant planets. However, the high-pressure phase diagram of even the simplest and most abundant elements hydrogen and helium as well as that of molecular systems (e.g. water, ammonia, methane and their mixtures) is not well known. The complexity of the behavior arises from metal-insulator transitions and demixing phenomena that occur at high pressures. New phases with exotic properties (e.g. superionic phases with proton conduction) have been predicted as well. These effects will have a strong impact on interior and dynamo models of solar and extrasolar giant planets.
We apply ab initio molecular dynamics simulations based on finite-temperature density functional theory to calculate the equation of state data, the high-pressure phase diagram, and the transport properties (electrical and thermal conductivity, viscosity) for a wide range of densities and temperatures. We present new results for hydrogen-helium mixtures and for water, ammonia, and methane. We discuss implications for the interior and magnetic field structure of the gas giants Jupiter and Saturn and the ice giants Uranus and Neptune.