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Metallization of dense fluid helium from ab initio simulations

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An earlier study [1] benchmarked Density Functional Theory (DFT) coupled with classical Molecular Dynamics (MD) with all available experimental data on dense helium in recent years. A subsequent study [2] calculated the helium melting line with DFT-MD. These two studies allows for the examination of the metallization of fluid helium consistently with DFTMD [3].
We study the insulator-to-metal transition at densities between 1 and 22 g/cm and
temperatures between 10 000 and 50 000 K. We calculate the equation of state, the band gap dependent on density and temperature by using different definitions [4-7], the DC conductivity, the reflectivity, and the ionization degree for which a novel method has been proposed recently [see M. Bethkenhagen et al., Phys. Rev. Res. 2, 023260 (2020)]. We find no indication of a first-order phase transition in any of the properties studied here and conclude that the metallization of fluid helium is continuous. For instance, we do not observe jumps in the DC conductivity and/or the reflectivity when the band gap closes.
However, the ionization degree increases from below 10% at the lowest to over 99% at the highest densities which reflects the continuous insulator-to-metal transition. The increase is almost exclusively driven by pressure ionization and shows only a weak temperature dependence.
We discuss the high-pressure phase diagram of helium and the implications of our results on the structure of astrophysical objects like gas giant planets and brown dwarfs.

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