ELECTRICAL CONDUCTIVITY OF WARM DENSE MATTER BASED ON DENSITY FUNCTIONAL THEORY: LOW-DENSITY BENCHMARKS AND VIRIAL EXPANSION INCLUDING ELECTRON-ELECTRON COLLISIONS

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Density functional theory based molecular dynamics simulations are a very successful tool to calculate the electrical conductivity of materials in the region of warm and dense matter. However, it requires a correction to implement the contribution of electron-electron collisions in the low-density, high-temperature region of plasmas. Based on the virial expansion of the electrical conductivity, a correction factor is presented, motivated by generalized linear response theory. For different materials, we identify the region in the temperature-density plane where the contribution of electron-electron collisions to the electrical conductivity is essential. In the range of low densities and high temperatures, the validity of the virial expansion is shown using the virial plot presentation.

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