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Ionization in high-density plasmas: an ab initio study for carbon at Gbar pressures

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We apply density functional theory molecular dynamics (DFT-MD) simulations to calculate the ionization degree of plasmas in the warm dense matter regime. Standard descriptions of the ionization potential depression (IPD) have been challenged recently by experiments approaching unprecedentedly high densities indicating that improved IPD models are required to describe warm dense matter. We propose a novel ab initio method to calculate the ionization degree directly from the dynamic electrical conductivity using the Thomas-Reiche-Kuhn
(TRK) sum rule. This
approach is demonstrated for carbon at a temperature of 100 eV and pressures in the Gbar range.
We find substantial deviations from widely applied IPD models like Stewart-Pyatt and Ecker-Kröll implying that condensed matter and quantum effects like band structure and Pauli blocking need to be included explicitly in ionization models. Our results will help to precisely model matter under conditions occurring, e.g., during inertial confined fusion implosions or inside astrophysical objects such as brown dwarfs and low-mass stars.

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