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First-Principles Determination of Electron-Ion Energy Relaxation Rates in the Warm Dense Matter Regime[1]

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The last decade has seen remarkable progress in our ability to create in the laboratory materials in the warm dense matter regime. These advances require improved understanding and forward modeling of the non-equilibrium conditions typically created in these experiments. In particular, much uncertainty remains in our predictive capability of the electron-ion energy relaxation timescales as illustrated by the strong disagreements among analytical models and with measurements. In this work [1] we present the first ab-initio calculations of the electron-ion energy relaxation rates in warm dense plasmas, liquid metals, and hot solids. To this end, we first derive a general expression for the rate and evaluate it numerically from quantum molecular dynamics simulations. Our theory includes self-consistently the various quantum, thermal, non-linear and strong coupling effects that coexist in warm dense plasmas, and it reduces to well-known models in limiting cases. We discuss results obtained for several representative materials, including H, Al, Cu, Ni and Fe, over a wide range of conditions. Our approach serves as a very useful comparison with experimental measurements and models, permits an extension into conditions not covered by experiments, and provides insight into the underlying physics. [1] J. Simoni and J. Daligault, First-Principles Determination of Electron-Ion Couplings in the Warm Dense Matter Regime, Phys. Rev. Lett. 122, 205001 (2019).

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