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Molecular dynamics simulations and generalized Lenard-Balescu calculations of electron-ion temperature relaxation in plasmas LORIN X. BENEDICT, MICHAEL P. SURH, SAAD A. KHAIRALLAH, JOHN I. CASTOR, HEATHER D. WHITLEY, DAVID F. RICHARDS, JAMES N. GLOSLI, LLNL, MICHAEL S. MURILLO, LANL, FRANK R. GRAZIANI, LLNL — We present classical molecular dynamics (MD) calculations of temperature relaxation in hydrogen, Ar-doped hydrogen, and SF_6 plasmas in which the two-particle interactions are represented by statistical potentials of the Dunn-Broyles and modified Kelbg forms. Using a multi-species generalized Lenard-Balescu theory in which the full frequency and wave-vector dependent dielectric response is included, we show that deviations of our hydrogen MD results from the weak-coupling theories such as Landau-Spitzer are due in large part to the use of the statistical potentials which approximate, in a classical way, the effects of quantum diffraction. Classical MD with Kelbg potentials is shown to be better at reproducing intermediate-to-weak-coupling results of true quantum-Coulomb plasmas, but it is also shown that MD with both types of statistical potential yield the correct quantum result in the limit of infinitesimal plasma coupling. Effects of dynamical screening in multi-component plasmas are also discussed.

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