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Coupled Ionic and Electronic Heat Transport at the Nanoscale¹ N.A. MODINE, R.E. JONES, J.A. TEMPLETON, G.J. WAGNER, D.L. OLM-STED, Sandia National Laboratories, R.M. HATCHER, Lockheed Martin Advanced Technology Laboaratory, M.J. BECK, University of Kentucky — In modeling thermal transport in nanoscale systems, classical molecular dynamics (MD) explicitly represents phonon modes and scattering mechanisms, but electrons and their role in energy transport are missing. Furthermore, the assumption of local equilibrium between ions and electrons often fails at the nanoscale. We have coupled MD (implemented in the LAMMPS MD package) with a partial differential equation based representation of the electrons (implemented using finite elements). The coupling between the subsystems occurs via a local version of the two-temperature model. Key parameters of the model are calculated using the Time Dependent Density Functional Theory with either explicit or implicit energy flow. We will discuss application of this work in the context of the US DOE Center for Integrated Nanotechnologies (CINT).

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