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Highly parallel implementation of non-adiabatic Ehrenfest molecular dynamics YOSUKE KANAI, The University of North Carolina at Chapel Hill / Lawrence Livermore National Laboratory, ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign / Lawrence Livermore National Laboratory, ERIK DRAEGER, Lawrence Livermore National Laboratory, VICTOR ANISIMOV, National Center for Supercomputing Applications, ALFREDO CORREA, Lawrence Livermore National Laboratory — While the adiabatic Born-Oppenheimer approximation tremendously lowers computational effort, many questions in modern physics, chemistry, and materials science require an explicit description of coupled *non-adiabatic* electron-ion dynamics. Electronic stopping, i.e. the energy transfer of a fast projectile atom to the electronic system of the target material, is a notorious example. We recently implemented real-time time-dependent density functional theory based on the plane-wave pseudopotential formalism in the Qbox/qb@ll codes. We demonstrate that explicit integration using a fourth-order Runge-Kutta scheme is very suitable for modern highly parallelized supercomputers. Applying the new implementation to systems with hundreds of atoms and thousands of electrons, we achieved excellent performance and scalability on a large number of nodes both on the BlueGene based "Sequoia" system at LLNL as well as the Cray architecture of "Blue Waters" at NCSA. As an example, we discuss our work on computing the electronic stopping power of aluminum and gold for hydrogen projectiles, showing an excellent agreement with experiment. These first-principles calculations allow us to gain important insight into the the fundamental physics of electronic stopping.

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