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A fast real time time-dependent density functional theory simulation method[1] LIN-WANG WANG, Lawrence Berkeley National Laboratory, ZHI WANG, Lawrence Berkeley National Laboratory, Berkeley; Institute of Semiconductors, Chinese Academy of Sciences, SHU-SHENG LI, Institute of Semiconductors, Chinese Academy of Sciences — We have developed an efficient real-time time-dependent density functional theory (TDDFT) method that can increase the effective time step from ¡1 attosecond in traditional methods to 0.1 0.5 femtosecond. Our algorithm, which carries out the non-adiabatic molecular dynamics TDDFT simulations, can have comparable speed to the Born-Oppenheimer (BO) ab initio molecular dynamics (MD). As an application, we simulated the process of an energetic Cl particle colliding onto a monolayer of MoSe2. Our simulations show a significant energy transfer from the kinetic energy of the Cl particle to the electronic energy of MoSe2, and the result of TDDFT is very different from that of BO MD simulations. This new algorithm will enable the use of real-time TD-DFT for many new simulations involving carrier dynamics and electron-phonon couplings.

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