A fast real time time-dependent density functional theory simulation method\textsuperscript{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 $\approx 1$ 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 MoSe\textsubscript{2}. Our simulations show a significant energy transfer from the kinetic energy of the Cl particle to the electronic energy of MoSe\textsubscript{2}, 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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