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Real-time electron dynamics for massively parallel excited-state simulations XAVIER ANDRADE, Lawrence Livermore National Laboratory, Livermore, CA — The simulation of the real-time dynamics of electrons, based on time dependent density functional theory (TDDFT), is a powerful approach to study electronic excited states in molecular and crystalline systems. What makes the method attractive is its flexibility to simulate different kinds of phenomena beyond the linear-response regime, including strongly-perturbed electronic systems and non-adiabatic electron-ion dynamics. Electron-dynamics simulations are also attractive from a computational point of view. They can run efficiently on massively parallel architectures due to the low communication requirements. Our implementations of electron dynamics, based on the codes Octopus (real-space) and Qball (plane-waves), allow us to simulate systems composed of thousands of atoms and to obtain good parallel scaling up to 1.6 million processor cores. Due to the versatility of real-time electron dynamics and its parallel performance, we expect it to become the method of choice to apply the capabilities of exascale supercomputers for the simulation of electronic excited states.

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