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Real-Time TDDFT simulation for coherent phonon generation in crystalline solids YASUSHI SHINOHARA, SHUNSUKE A. SATO, KAZUHIRO YABANA, University of Tsukuba, TOMOHITO OTOBE, Japan Atomic Energy Agency, JUN-ICHI IWATA, University of Tokyo, GEORGE F. BERTSCH, University of Washington — We have been developing a theoretical framework to describe electron dynamics in a crystalline solid under an ultrashort laser pulse. We rely upon the time-dependent density functional theory, solving the time-dependent Kohn-Sham equation in real-time and real-space. Using our method, it is possible to describe both linear and nonlinear light-matter interactions in a unified way. In my presentation, I will focus on the application to coherent phonon generation, a coherent atomic oscillation over a macroscopic volume. I will show applications to two material, semiconductor Si and semimetal Sb. For Si, we have found that the TDDFT is capable of describe two distinct mechanisms of the coherent phonon generation. When the laser frequency is below the direct bandgap, virtual electronic excitation induces impulsive force to atoms. When the laser frequency is above the gap, real electronic excitation causes the atomic motion. For Sb, we study the frequency dependence of the coherent phonon generation and compare our results with phenomenological theories.

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