Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

AB INITIO DYNAMICS OF AN ELECTRON INTERACTING WITH A LATTICE DEFECT VSEVOLOD IVANOV, MARCO BERNARDI, California Institute of Technology, Pasadena, California 91125. — We study the scattering process of a charge carrier with a defect in a range of bulk and 2D materials. The scattering potential is obtained using density functional theory, the carrier is represented by a gaussian wavepacket, and the dynamics is carried out with a split-operator technique. Our parallel code can model the electron-defect scattering processes in real space and time, with an electron wavepacket of realistic size (100 - 1000 unit cells) and an accuracy typical of ab initio calculations. We apply our approach to model a carrier scattering with a vacancy in silicon and an impurity in monolayer MoS2, obtaining angular dependent scattering cross sections and resonant states.

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Date submitted: 04 Nov 2015 Electronic form version 1.4