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Charge Carrier Scattering with Defects from First-Principles Calculations I-TE LU, JIN-JIAN ZHOU, LUIS AGAPITO, MARCO BERNARDI, Caltech — Phonons and defects are the main sources of charge carrier scattering in materials. While first-principles electron-phonon calculations are being actively studied, electron-defect scattering has not been explored extensively from first principles. Scattering due to defects is important both because defects are naturally present in materials and because it limits carrier mobility at low temperature, and at room temperature in highly doped samples. We discuss the formalism to compute electron-defect scattering from first principles. The main quantities in the calculation are the matrix elements of the defect perturbation potential in a Kohn-Sham basis. Both the local perturbation potential due to electrons and ions and the nonlocal contribution from the pseudopotential are considered. We interpolate these matrix elements on fine girds to calculate the carrier relaxation time and low temperature mobility in silicon due to elastic scattering with neutral defects, such as vacancies and Frenkel pairs, using Fermis golden rule and the Born approximation. The development of efficient parallel algorithms for electron-defect calculations is also discussed.

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