Highlights

RESEARCH AREA 3 - Quantum Science and technologies - 2022

"Electron-Phonon Interaction and Longitudinal-Transverse Phonon Splitting in Doped Semiconductors"

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Electron-phonon interactions (EPI) shape many physical properties of condensed matter, from transport and optical properties to superconductivity. In polar semiconductors, the long-range Coulomb-mediated Fröhlich interaction dominates in the long wavelength limit, causing a splitting of longitudinal (LO) and transverse (TO) optical phonon modes and strongly affecting chargecarrier lifetimes. We study the impact of electron screening on the Fröhlich interaction in doped semiconductors by introducing a momentum-dependent generalization of Born effective charges (BECs), measuring the dipole moments of optical phonons. Our linear-response formulation, rooted in Density Functional Perturbation Theory, enables to treat screening effects via controlled approximations on the dielectric function, while evaluating ab initio in the undoped setup all other quantities contributing to the dielectric response. As an illustrative case, we study EPI and the LO-TO splitting of doped cubic silicon carbide. We further evaluate the electronic lifetime due to the EPI with LO phonons, often limiting intrinsic carrier mobility of polar doped semiconductors. Our work highlights the need of including free-carriers screening for a proper assessment of transport properties in doped semiconductors. The proposed approach for dealing with electronic screening lays the foundation for further extensions tackling other less conventional types of electron-phonon interactions, as well as giving access to the vibrational contribution to the full macroscopic dielectric function that shapes the dynamical structure factor probed in inelastic scattering experiments.

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Fig. 1: (Left) Momentum-dependent BECs of Si and C in 3C-SiC along the highsymmetry red line displayed in the Brillouin zone for the undoped (empty circles) and doped case for a hole carrier concentration of $p = 4.827 \times 10^{15} \text{ cm}^{-3}$ (full squares). (Right) LO and TO phonons and EPI in undoped (empty circles) and doped (full square) setup, highlighting the strong screening effect onto LO quantities. The as linewidths in left and central panel and in vertical black line is drawn at the effective Fermi momentum k_{F} .

Fig. 2: Inverse lifetime scattering due to LO phonons evaluated with (light blue) and without (light gray) including screening effects for a hole concentration $p \sim 10^{20} \text{ cm}^{-3}$, shown absolute magnitude in right panel.



