Effective charges, electron-phonon interaction and infrared spectroscopy in doped semiconductors, metals and hydrogen-based high-Tc superconductors

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Electron-phonon coupling and phonon frequencies of polar semiconductors are sensitive to the long-range Coulomb interactions and can therefore be strongly affected by free-carrier screening, with significantly different behaviours as a function of the dimensionality. We show within a linear-response dielectric-matrix formulation that the interplay between polarization and screening can still be described even in presence of doping by appropriate momentum dependent effective charges functions and the inverse scalar dielectric function. In this way, it is possible to obtain the three and two dimensional generalization of the Frölich-like interaction vertex and of the Born-Huang theory of polar crystal lattices to the cases where polarization seemingly cannot be defined. As a by-product of our developments, we can also access the infrared spectrum of bad metals—such as superhydrides—which depends on both adiabatic (static) and non-adiabatic (dynamical) Born effective charges, opening up the opportunity to precisely characterize the phonon resonances of promising superconductors. From an operative point of view, we propose computational methods to evaluate from first principles both effective charge functions – encompassing all multipolar components beyond dynamical dipoles and quadrupoles – and the static dielectric function of two-dimensional semiconductors, with approaches based on perturbation theory and on Wannier interpolation techniques.

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