Electron-Phonon Interactions in Piezoelectric Crystals and the Missing Quadrupole Term

Jhalani, Vatsal A. and Zhou, Jin-Jian and Park, Jinsoo and Dreyer, Cyrus E. and Bernardi, Marco. *Piezoelectric Electron-Phonon Interaction from Ab Initio Dynamical Quadrupoles: Impact on Charge Transport in Wurtzite GaN (2020)* Physical Review Letters, 125 (13). DOI: 10.1103/PhysRevLett.125.136602

Scientific Achievement

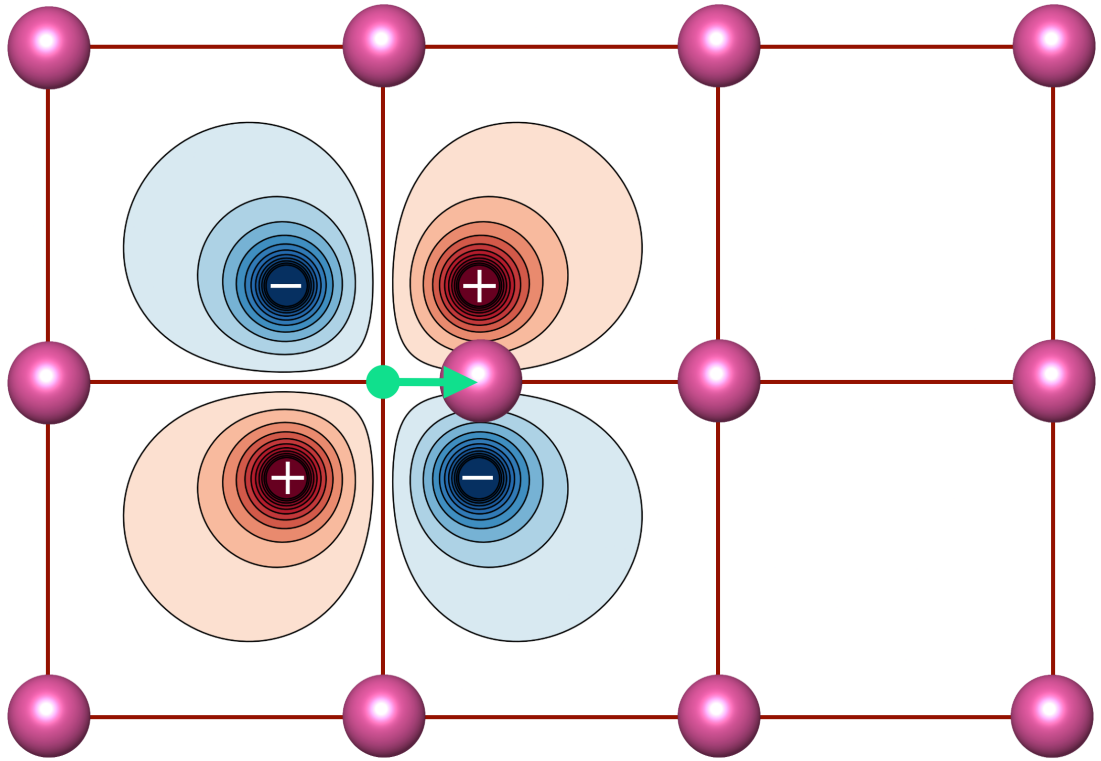
- Development of a more accurate computational method to study the electron dynamics in piezoelectric (PE) materials.

Significance and Impact

- A quantitative framework enabling accurate calculations of long-range interactions between electrons and lattice vibrations in PE materials.

Technical Details

- The framework computes the e-ph interaction due to the quadrupole term.
- Applied to wurtzite GaN, a PE crystal, and showed all short- and long-range interactions between electrons and phonons are accurately captured.



Due to thermal atomic motions, electrons in a material feel changes in their potential energy due to both short-range and long-range electrostatic forces. An intermediate type of long-range electron-phonon (e-ph) interaction arises in piezoelectric crystals, where strain induced by acoustic phonons results in quadrupole-like potential terms. Our quantitative framework computes the e-ph interaction due to the quadrupole term for more accurate studies of electron dynamics in PE.
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