# Phonon-mediated quantum processes in semiconductors

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Quantum processes between electrons, excitons, phonons, and photons play a critical role in the operation of electronic and optoelectronic semiconductor devices. While many of these processes are direct and can be accurately treated with first-order perturbation theory, others, such as optical transitions in indirect-gap materials, are enabled only by the additional momentum provided by phonons, necessitating a higher-order treatment that increases computational complexity. I will present our work on the development and application of first-principles computational methods to study phonon-mediated quantum processes in semiconductor materials. I will first discuss how phonons enable light absorption in technologically important indirect-gap materials such as silicon [1], but also how they introduce free-carrier absorption that causes optical loss of sub-band-gap photons in doped semiconductors [2]. Additionally, I will demonstrate the critical role of phonons in enabling Auger-Meitner recombination in semiconductors—an important non-radiative electron-hole recombination mechanism that limits the quantum efficiency of devices such as solar cells or light emitters [3]. Last, I will discuss how screening of electron-hole Coulomb attraction by phonons is affected by quantum confinement in atomically thin semiconductors [4]. Our work demonstrates the important role of predictive atomistic calculations in quantitatively understanding phonon-mediated quantum processes in modern electronic and optoelectronic semiconductor devices.

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[2] *Phys. Rev. B* **106**, 205203 (2022)
[3] *Phys. Rev. Lett*. **131**, 076902 (2023); *Appl. Phys. Lett*. **125**, 021109 (2024).
[4] *Phys. Rev. Lett*., in press (arXiv:2408.00924)