School of Nano Science

PhD Defense

Properties of electron-phonon interaction in 2D crystal structures

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Abstract:

Density Functional Theory (DFT) as a first principles method is capable to calculate almost all the quantities that are necessary to estimate electron-phonon matrix elements used to evaluate different quantities such as superconducting transition temperature, Kohn anomaly and damping rate of the plasmon frequency. Therefore, in this work, a comprehensive investigation of a possible superconducting phase in the monolayer indium selenide is done by using DFT calculations for both hole and electron doped systems. The hole doped dependence of the Fermi surface is exclusively fundamental for the monolayer InSe. It leads to the extensive modification of the Fermi surface from six separated pockets to two pockets by increasing the hole densities. For quite low hole doped of the system, below the Lifshitz transition point, a strong electron-phonon coupling $\lambda \sim 7.5$ is obtained; uniquely determining a superconductive critical temperature as high as Tc∼55−75 K depends on different amounts of effective Coulomb potential from 0.2 to 0.1. However, for some hole doping above the Lifshitz transition point, the combination of the temperature dependence of the bare susceptibility and the strong electron-phonon interaction gives rise to a charge density wave that emerged at a temperature far above Tc. Having included non-adiabatic effects, we could carefully analyze conditions for which either a superconductive or charge density wave phase occurs in the system. In notable addition, monolayer InSe becomes dynamically stable by including non-adiabatic effects for different carrier concentrations at room temperature. Another work includes the effects of spin-orbit (SOC) and electron-phonon coupling on the collective excitation of doped monolayer Sb2 by using density functional and many body perturbation theories. The spin-orbit coupling is exclusively important for the monolayer Sb_2 and it leads to the modification of the electronic band structure. In particular, plasmon modes of monolayer Sb_2 are quite sensitive to the SOC and are characterized by very low damping rates owing to small electron-phonon scatterings. Our results show how plasmons in antimonene are significantly less damped compared to monolayer graphene when plasmon energies are larger than 0.2 eV due to smaller plasmon-phonon coupling in the former material.

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