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Possible superconductivity of WS₂: An Abinitio study

Abstract

Recently, searching for possibility of superconducting properties in low dimensional materials has been attracted intense interest. In the present work, we have investigated the electronic properties and possibility of superconductivity in bulk and atomically thin WS₂ using *ab initio* calculations. We have systematically examined the semiconductor to metallic transition upon carrier doping on bulk and monolayer WS₂. Both electron and hole doping influence the electronic properties of WS₂ and transform from semiconductor to metallic nature. Our results show that the pristine single layer WS₂ is a semiconductor with the direct band gap and the electronic properties of WS₂ are similar those of MoS₂. However, notable changes in the phonon spectra were observed with the external stimuli, which may induce the superconductivity in both bulk and single layer WS₂. We calculated the electron-phonon coupling, critical temperature (T_c), and influence of Coulomb interaction (μ^*) on T_c, using isotropic Migdal-Eliashberg theory with the combination of Wannier-Fourier interpolation. Our results provide that the carrier doping is the only scenario to induce superconductivity, which is consistent with the recent ion-gate experiments.