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Quasiparticle Band Gap Renormalization in Doped Two-Dimensional Materials[1] YUFENG LIANG[2], Lawrence Berkeley National Lab, LI YANG, Department of Physics, Washington University in St. Louis — Recently, atomically thin two-dimensional (2D) materials have emerged as new prototypes for a variety of electronic and optoelectronic devices, for which charge carrier doping is an effective approach for modifying their intrinsic properties. In the process of producing monolayer metal dichalcogenides, doping can occur naturally and may lead to exotic many-body phenomena as evidenced in recent optical experiments. Despite the common occurrence of doping in 2D structures, little knowledge has been obtained for the evolution of the band gap with the carrier concentration, which is key to harnessing the electronic properties and understanding more complicated many-body effects. Here, we investigate how the band gap changes with doping density in various 2D structures. Based on the conventional GW method for semiconductors, we devised and implemented an efficient calculation scheme to capture the unique dielectric screening arising from intraband transitions in low-dimensional structures, specifically MoS2 and MoSe2. We reveal that an enhanced band gap renormalization of a few hundred meV can be achieved and the band gap evolution displays an unusual nonlinear behavior with doping density. Our calculated band gap is in excellent agreement with the recent ARPES experiments on MoSe2.

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