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Enhanced quasiparticle band gap renormalization in doped two-dimensional semiconductors LI YANG, SHIYUAN GAO, Department of Physics, Washington University in St Louis, YUFENG LIANG, Lawrence Berkeley National Lab — One of the most prominent features of two-dimensional (2D) materials is the enhanced many-body interactions because of quantum confinement and reduced electronic screening. Doping is widely observed in 2D materials by either inevitable defects or intended electrostatic and chemical processes. The doped free carriers introduce additional screening and plasmon excitations, which substantially modifies many-body interactions. This factor and enhanced van Hove singularities lead to a large, nonlinear quasiparticle band gap renormalization (BGR) in 2D semiconductors. Using the GW approximation, we developed an efficient scheme to calculate the BGR by separating the doping contributions to the quasiparticle self-energy from the intrinsic one. Based on our first-principles calculation, we report enhanced BGR (a few hundred meV) of monolayer transition metal dichalcogenides, black phosphorus, and hexagonal BN. Our result is crucial for interpreting experimental measurements and quantitatively understanding and engineering quasiparticle band gaps in 2D semiconductors.

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