Obtaining Excited-State Properties in Doped Two-Dimensional Materials with an Efficient Plasmon-Pole Model

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Determining electronic excitations from first-principles calculations greatly facilitates the designs of functioning materials in electronics and opto-electronics. For systems with medium electron correlations, the key often lies in a successful modeling of the screened Coulomb interactions among the charges. In general, this procedure is formidable since the dielectric screening varies drastically across different length-scales and time-scales. Recently, layered metal dichalcogenides emerge as a novel class of two-dimensional devices, where doping is an important means of controlling their physical properties effectively. From the perspective of first-principles simulations, extra carriers add to the complexity of modeling the dielectric function. In this work, we propose a generic and efficient dielectric model for doped low-dimensional materials [1]. It is found that at commonly seen doping levels, the extra charge carriers only affect the long-wave components of the dielectric function while the other components remain largely intact. The charge carriers contribute to the formation of a lower-energy plasmon, which can be shown to be captured by undemanding computational efforts. Using the GW approximation, we apply our model to the quasiparticle band energies in MoS_2 and $MoSe_2$ and achieve excellent agreement with recent ARPES experiments. This model can also be further applied to the Bethe-Salpeter Equation for electron-hole excitations.

[1] Yufeng Liang and Li Yang, Phys. Rev. Lett. 114, 063001 (2015)