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Dynamical Excitonic Effects in Doped Two-Dimensional Semiconductors[1] SHIYUAN GAO, Department of Physics, Washington University in St. Louis, YUFENG LIANG, Lawrence Berkeley National Laboratory, CATALIN SPATARU, Sandia National Laboratory, LI YANG, Department of Physics, Washington University in St. Louis — It is well-known that excitonic effects can dominate the optical properties of two-dimensional materials. These effects, however, can be substantially modified by doping free carriers. We investigate these doping effects by solving the first-principles Bethe-Salpeter Equation. Dynamical screening effects, included via the sum-rule preserving generalized plasmon-pole model, are found to be important in the doped system. Using monolayer MoS_2 as an example, we find that upon moderate doping, the exciton binding energy can be tuned by a few hundred meVs, while the exciton peak position stays nearly constant due to a cancellation with the quasiparticle band gap renormalization. At higher doping densities, the exciton peak position increases linearly in energy and gradually merges into a Fermi-edge singularity. Our results are crucial for the quantitative interpretation of optical properties of two-dimensional materials and the further development of ab initio theories of studying charged excitations such as trions.

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