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Ab Initio Study of Quasiparticle and Excitonic Properties of MoS2 DIANA QIU, FELIPE JORNADA, STEVEN LOUIE, UC Berkeley and Lawrence Berkeley National Lab — MoS2 is a layered, transition-metal dichalcogenide that can be cleaved into single-layer sheets, in a manner similar to graphene. Monolayer MoS2 has a direct band gap, strong spin-orbit coupling and strongly enhanced photoluminescence, compared with the bulk. MoS2's interesting electronic and optical properties mean that it could have many applications in single-layer electronic devices, but on the theoretical level, when many-electron interaction effects are included, there is still some uncertainty about the quasiparticle and excitonic properties of MoS2. We use first-principles calculations to study the quasiparticle band structure and optical absorption spectrum of MoS2 at the GW+BSE level. We include spin-orbit coupling as a perturbation either before or after the GW calculation of the band structure, and we demonstrate that our calculations are fully converged with respect to the dielectric cutoff and summation over empty bands. This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC.

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