Quasiparticle Band Structure Calculation of Monolayer, Bilayer, and Bulk MoS_2

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Quasiparticle self-consistent *GW* calculations of the band structures and related effective mass parameters are carried out for bulk, monolayer and bilayer MoS_2. Including excitonic effects within the Mott-Wannier theory, quantitative agreement is obtained between the A, B excitons, measured by absorption [1], and the calculated exciton gap energies at K. The A-B splitting arises from the valence band splitting which in the monolayer is entirely due to spin-orbit coupling and leads to spin-split states, while in the bilayer it is a combined effect of interlayer and spin-orbit coupling.

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[1] K. F. Mak, C. Lee, J. Hone, J. Shan, and T. F. Heinz, Phys. Rev. Lett. **105**, 136805 (2010).

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