Optical spectra of MoS_2: dependence on substrate and electron-phonon coupling

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Layered transition-metal dichalcogenides, in particular the semiconducting MoS_2, are attracting currently a lot of attention due to their possible use in thin-film electronics. Also from the fundamental point of view, these materials are very interesting due to their complex band-structure, strong effects of spin-orbit splitting and the possibility of valley polarization by circularly polarized light. We summarize the debate on the quasi-particle band-structure of single and few-layer MoS_2 (self-consistent versus non-self consistent GW). We discuss the influence of slight changes in the geometry of the single-layer as well as of the underlying substrate. Optical absorption spectra are calculated on the level of the Bethe-Salpeter equation including the effect of spin-orbit coupling. Taking into account the effect of electron-phonon coupling, we calculate the temperature dependence of the band gap and the absorption spectra. We discuss the origin of the experimentally observed doubling of the high-energy exciton at 2.6 eV on a gold substrate as the potential effect of a "mirror exciton" (exciton formed from image states).

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