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Substrate-induced renormalization of the quasiparticle and optical gaps in monolayer transition metal dichalcogenides from GW and GW-BSE calculations. FELIPE H. DA JORNADA, CHIN SHEN ONG, DIANA Y. QIU, STEVEN G. LOUIE, UC Berkeley and Lawrence Berkeley National Lab — There has been a considerable effort to experimentally characterize the electronic and optical properties of novel atomically thin 2D semiconductors, such as mono- and few-layer transition metal dichalcogenides (TMDs). However, the role that different substrates play in these experiments still remains unclear. From a theoretical perspective, it is hard to include the substrate in an *ab initio* framework, while in experiments, it is often difficult to suspend these samples. Here, we present a new method to compute the substrate effect on the quasiparticle and optical properties of quasi-2D materials based on state-of-the-art *ab initio* GW and GW plus Bethe-Salpeter equation (GW-BSE) methods. We compute the effects of different metallic and semiconducting substrates, and show that the quasiparticle gap and exciton binding energy can be dramatically reduced even with semiconducting substrates. This work was supported by the National Science Foundation under Grant No. DMR15-1508412 and the DOE under Contract No. DE-AC02-05CH11231.

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