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The influence of composition and mechanical strain on the optoelectronic properties of transition-metal dichalcogenide monolayers ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst — Single and few-layer transition-metal dichalcogenides (TMDs) are of significant current interest for nanoscale optoelectronic applications. While these materials have been well characterized in their bulk form, a comprehensive understanding of their properties at the nanoscale is still emerging. We present studies of the quasiparticle band structures and optical properties of MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2 monolayers using the GW approximation in conjunction with the Bethe-Salpeter equation (BSE). The inclusion of two-particle excitations in the BSE approach reveals the presence of two strongly bound excitons (A and B) below the quasiparticle absorption onset arising from vertical transitions between a spin-orbit-split valence band and the conduction band. The transition energies for monolayer MoS_2, in particular, are shown to be in excellent agreement with available experiments. Excitation energies for the remaining monolayers are predicted to lie in the range of 1–2 eV. Systematic trends are identified for band gaps, transition energies, and exciton binding energies within as well as across the Mo and W families of dichalcogenides. Finally, we study the influence of homogeneous strains on the optoelectronic properties of TMD monolayers and demonstrate the potential for facile tuning of electronic and optical band gaps. Overall, the results suggest that quantum confinement of carriers within monolayers can be exploited in conjunction with chemical composition and mechanical strains to widely tune the optoelectronic properties of TMDs at the nanoscale.

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