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Characterizing and tuning excitons in monolayer and few-layer MoS_2[1] DIANA Y. QIU, FELIPE H. DA JORNADA, STEVEN G. LOUIE, Univ of California - Berkeley and Lawrence Berkeley National Lab — We use the GW-BSE method to study excitons arising from transitions in different regions of momentum space in mono- and few-layer MoS_2 and consider mechanisms to fundamentally change the features and character of the optical spectra. Our calculations show that sharp spatial variations in dielectric screening make 2D systems, such as MoS_2, computationally challenging, requiring very fine k-space sampling to resolve the structure of excitonic wave functions and converge binding energies. In highly converged calculations, we identify a series of excitons arising from transitions at the K/K$'$ valleys in the Brillouin zone, a higher energy series arising from transitions in the valley of a Mexican hat potential centered at the Γ point, and transitions at the indirect gap from Γ to Λ in few-layer MoS_2. As layer number changes, these states, which have varying character, momentum-space structure and real-space locations, are affected differently by changes in confinement and hybridization. By tuning layer number and strain, we find that we not only can tune the excitation energies but can also change the relative energies of the various excitonic series, allowing for movement of the lowest energy exciton between different regions of the Brillouin zone

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