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Tuning excitons in monolayer and few-layer MoS₂¹ DIANA Y. QIU, FELIPE H. DA JORNADA, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Our recent ab initio GW-BSE calculations showed that monolayer MoS₂ is a computationally challenging system, requiring a large number of empty bands and very fine k-point sampling to converge its quasiparticle band structure and optical properties. Careful convergence of a GW-BSE calculation reveals that MoS₂ has a large number of bound excitons with varying k-space characteristics. Specifically, there are two series of excitons: a low-energy series with k-space wavefunctions localized at the K/K' valleys in the Brillouin zone and a higher energy series localized in a ring around the Γ point. There is very little hybridization between these two exciton series in monolayer MoS₂, but changes in electronic structure and screening due to additional layers, strain, or doping can lead to changes in exciton binding energies, character, and hybridization. Thus, we have carried out ab initio GW-BSE calculations to study the excitonic properties of few-layer MoS₂. We find that layering and straining MoS₂ systematically changes the exciton binding energies, the peak positions and amount of absorbance in the optical spectrum, and the character and hybridization of the excitons near Γ .

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