

Abstract Submitted
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Temperature Effects on Optical Spectra of Monolayer MoS₂¹ LI YANG, Washington University in St Louis — We present the effects of temperature on the electronic structure and optical spectra of monolayer MoS₂. Newly measured optical absorption and photoluminescence spectra reveal substantial frequency shifts of exciton peaks as monolayer MoS₂ is cooled from 300 K to 4 K. First-principles simulations using the GW-Bethe Salpeter Equation approach satisfactorily reproduce these frequency shifts by incorporating the thermal expansion. Studying these temperature effects in monolayer MoS₂ is crucial for rectifying the results of room-temperature experiments with the previous predictions of zero-temperature-limit simulations. Additionally, we show that tracking the frequency shifts in the exciton peak of optical spectra may serve as a convenient way of estimating thermal expansion coefficients in two-dimensional chalcogenides.

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