Abstract Submitted
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First-principles Study of Temperature Dependence of Energy Gap in 2D Materials[1] YUNING WU, XIAOGUANG ZHANG, Department of Physics and Quantum Theory Project, University of Florida — We use a first-principles method to study the temperature dependence of energy gap in 2D semiconductors, including monolayer MoS_2 and $MoSe_2$, *etc*, due to the effect of phonons on the band structure. The phonon vibrations are modeled by a set of frozen-phonon configurations, in which atomic displacements are determined by the Bose-Einstein distribution of the phonon modes. The electronic structure is calculated for each configuration, and the energy gap is extracted from configurational statistics. Calculated temperature dependence of energy gap agrees with the photoluminescence experiments [1] in terms of both the values of the band gap as well as the line shapes.
[1] S. Tongay *et al.*, Nano Lett. 12, 5576, (2012)

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