

Abstract Submitted
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Resonance Raman intensities including excitonic effects from first-principles: application to 2D materials YUANXI WANG, AMBER MC-CREARY, Pennsylvania State University, JEFFREY SIMPSON, NIST, DANIEL RHODES, LUIS BALICAS, Florida State University, MAURICIO TERRONES, Pennsylvania State University, ANGELA WALKER, NIST, VINCENT CRESPI, Pennsylvania State University — Recent advances in Resonance Raman (RR) spectroscopy on 2D semiconductors such as monolayer MoS₂ and ReS₂ discovered a rich variety of frequency- and polarization-dependent Raman signatures. Although the theory for RR has been well developed for the case of graphene, strong excitonic effects present in 2D semiconductors call for further scrutiny on Raman intensities based on first-principle calculations. Compared to existing methods of calculating RR intensities based on finite differences where the Bethe-Salpeter equation (BSE) was solved twice for each degree of freedom, we present a perturbational approach in which the BSE is only solved once statically and can be implemented to model first- and second-order resonance Raman processes. Comparisons with experimental results are discussed, as well as the connection between the finite differences and perturbational approaches.

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