

Symmetry-dependent exciton-phonon coupling in MoS₂/WS₂ heterostructure from first-principles analysis of resonant Raman spectrum

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Resonant Raman process involves inelastic scattering between photons and the electron-phonon system, in which an electron absorbs a photon and is excited to an excited state then jumps back to the ground state immediately by emitting another photon, and simultaneously emitting a number of phonons. We show that this process is properly described by a second-order Feynman diagram that is enabled by the Franck-Condon principle, which assumes instantaneous electron transition and slower ion relaxations. Our theory is applied to MoS₂/WS₂ bilayer system and yields a Raman spectrum that is compared to experiments.