Raman scattering of two-dimensional magnetic transition metal dichalcogenides

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The present theoretical study is devoted to first-principles calculations of the magnetic transition metal dichalcogenide (TMD) VS_2 within the framework of density functional theory. VS_2 is a distinctive TMD that exhibits intrinsic room-temperature ferromagnetism and metallic-to-semiconducting behavior depending on the structural phase [1, 2]. Despite the intensive research activity devoted to magnetic TMDs in recent years, driven by their promising prospects for applications in spintronics, straintronics, and optoelectronics, detailed theoretical studies of the Raman spectra of VS_2 as a function of the number of layers are still lacking. Thus, for VS_2 with different numbers of layers, the evolution of the positions of Raman-active vibrational modes, as well as the electronic band structure and magnetic properties, is investigated. Although the trends in Raman peak shifts remain similar as the number of layers changes, each number of layers corresponds to a unique Raman spectrum. Therefore, theoretical studies of Raman spectra not only provide insight into the vibrational properties of this material, but also enable unambiguous interpretation of experimental spectra and reliable determination of the number of layers.

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