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Optical Characteristic Study of Monolayer VS₂ Based on First-Principles Calculations

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Abstract: Monolayer VS₂ has two common stable phases, 2H-phase and 1T-phase. Based on first-principles calculations, we studied the optical properties of 2D-VS₂, including their dielectric functions, absorption coefficients, refraction indexes and energy loss functions. Also, we fully analyzed the relationship between the electronic structure and the optical characteristics of 2D-VS₂. We found that the differences of density of states are the fundamental reasons for the differences of the two phase optical absorption behavior.

Keywords: Two-dimensional materials; VS₂; first-principles calculations; optical properties

1. Introduction

Since the discovery of Graphene, research of two-dimensional (2D) materials has developed rapidly. Different kinds of interesting features gradually emerged and soon were applied in digital devices [1]. Two-dimensional transition metal dichalcogenides (TMDs) are one of the most studied materials among them [1,2], its special semiconductor band structure and density of states make it have a great potential value in the manufacture of lithium-ion batteries, flexible electronic devices, optical devices and low-power electronic devices etc. [1]. Monolayer VS₂ is very outstanding in TMDs, because it not only has electrical but also ferromagnetic properties, which make it could be applied in electromagnetic devices and nano-devices [3], and become one of the widely studied materials in TMDs.

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