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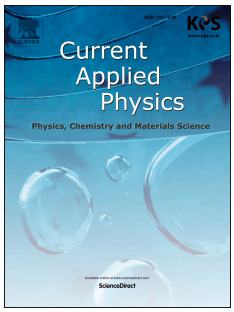

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First-principles study on the Poisson's ratio of transition-metal dichalcogenides

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Abstract

In this study, we investigate the Poisson's ratio of transition-metal dichalcogenides (TMDCs) with a chemical formula of MX_2, where M = Mo, W and X = S, Se, respectively, from first-principles. Through density functional theory calculations, it is demonstrated that the Poisson's ratio of MX_2 exhibits not only a substantial difference between the planar and vertical values but also a systematic dependence on the chalcogen species. Among the TMDCs, MoS_2 displays the strongest anisotropy, which entails a distinctive contracting response under a planar strain. We find that such pronounced anisotropy in the Poisson's ratio of the TMDCs originates from the different filling of the in- (p_x, p_y, d_{xy}, and $d_{x^2-y^2}$) and out-of-plane (p_z, d_{yz}, d_{zx}, and d_{z^2}) electronic orbitals depending on the transition-metal elements. These findings shed a new light on the elastic properties of TMDCs which continue to be interesting and show intriguing phenomena.

Keywords: Transition-metal dichalcogenides, Poisson's ratio, density functional theory, anisotropy

1. Introduction

Successful isolation of graphene from graphite through mechanical exfoliation has brought about tremendous interest in layered materials such as group-IV or -V elemental structures [1, 2, 3, 4, 5] and transition-metal-based compounds including transition-metal dichalcogenides (TMDCs) [6, 7]. The interest in these reduced-dimensional materials is primarily due to their rich and fascinating physics such as unique electronic structures, high mechanical strength and enhanced optical absorption, which also holds great promise for technological applications. Among them, TMDCs, which are denoted as MX_2 with M and X being transition-metal and chalcogen elements, respectively, have drawn particular attention because diverse electronic states, ranging from, for instance, semiconducting, metallic to superconducting ones, can be realized simply by varying chemical compositions [8]. In addition, within a given TMDC the electronic structure shows a distinctive layer-dependence in that the band gap of a semiconducting TMDC can be tuned by modifying the number of component X-M-X layers [9, 10, 11, 12, 13], which, together with the layer-dependent transition from indirect to direct gap, makes TMDCs particularly attractive for optoelectronic as well as electronic applications.

Mechanical aspects of TMDCs are of great interest as well since the electronic and optical