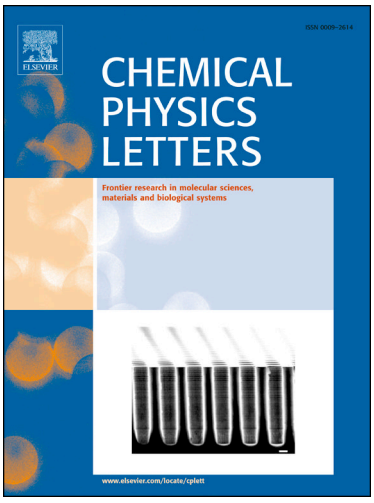

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Density functional theory study of inter-layer coupling in bulk tin selenide

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Abstract

We study the inter-layer coupling in bulk tin selenide (SnSe) through density functional theory based calculations. Different approximations for the exchange-correlation functionals and the van der Waals interaction are employed. By performing comparison with graphite, MoS_2 and black phosphorus, we analyze the inter-layer coupling from different points of view, including the binding energy, the low frequency inter-layer optical phonons, and the inter-layer charge transfer. We find that, there is a strong charge transfer between layers of SnSe, resulting in the strongest inter-layer coupling. Moreover, the charge transfer renders the inter-layer coupling in SnSe not of van der Waals type. Mechanical exfoliation has been used to fabricate mono- or few-layer graphene, MoS_2 and black phosphorus. But, our results show that it may be difficult to apply similar technique to SnSe.

Keywords: `2D materials, Inter-layer interaction, Density functional theory, Phonon spectrum`

1. Introduction

Since the discovery of graphene[1], two-dimensional (2D) materials and their hetero-structures have received considerable attention in many research fields, from basic science to engineering. Their single and few layers could be made either bottom-up using chemical synthesis or top-down by mechanical exfoliation. Due to the low cost and high quality output, mechanical exfoliation