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The Pyrite Structure of PdS_2 and $PdSe_2$ Monolayers ARUNIMA K. SINGH, National Institute of Standards and Technology, RICHARD G. HENNIG, University of Florida, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY COLLABORATION, UNIVERSITY OF FLORIDA COLLABORATION
— There has been a rising interest in two-dimensional (2D) materials due to a range of extraordinary electronic, optical and mechanical properties which are different from their bulk counterparts. The structure, stability and electronic properties of 2D PdS_2 and $PdSe_2$ have been investigated in the past in the well-known hexagonal 1T and 2H structures. However, bulk PdS_2 and $PdSe_2$ are layered compounds with individual rhombohedral pyrite-type monolayers vertically stacked with van-der Waals forces. Using density functional theory simulations, and five different functionals, we compare the energetic stability of 2D PdS_2 and $PdSe_2$ pyrite structure with the 1T and 2H structures. We find that the PdS_2 is most stable in the pyrite structure, whereas the $PdSe_2$ is most stable in the 1T structure with the pyrite structure closely competing in energy. The fundamental band gap of these compounds as a function of the structure, number of layers, the stacking arrangement and in-layer strain has been investigated. The pyrite structures of PdS_2 and $PdSe_2$ are found to be semi-conducting with indirect band gaps, and effective masses comparable to that of monolayer MoS_2; thus are potential candidates for nano-electronic applications.

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