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Band Gap Modulation by Two-Dimensional h-BN Nanostructure

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Two-dimensional hexagonal boron nitride (h-BN) as a graphene-like material was investigated due to its impending applications in electronics. The h-BN band gap E_g as an important factor and its variation between bilayer $ZrSe_2$ sheets were explored under an external electric field. The initially indirect band gap is found to convert to direct band gap by means of density functional theory. Additionally, the band gap is modulated by van der Waals corrections from 0.21220 eV to 0.01770 eV. Based on the results, the proposed heterostructure is converted to the direct band gap, and band gap smoothly decreased from 0.25440 eV to 0.0436 eV following the application of external electric field from 0.2 eV to 0.6 eV. Moreover, $ZrSe_2$|h-BN|$ZrSe_2$ is investigated under the applied biaxial compressive strain from 1% to 4%. The findings demonstrated that the gap was decreased by any compressive strain amplification, while the semiconducting behavior in the heterostructure attained to the semi-metallic performance under the increasing strain.

Keywords: Band gap modulation, h-BN, Nanostructure, Zirconium Diselenide