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Ab-initio study of structural and electronic properties of WS_2/h-BN van der Waals heterostructure

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Highlights

- WS2 monolayer is physisorbed on and between h-BN layers.
- Based on DFT calculations, the vdW-DF2B86R functional predicts the most accurate results.
- The WS_2/h-BN and h-BN/WS_2/h-BN systems have direct band gap at K-point.

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