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## **Supplementary Material**

## Calculations tunable electronic and optical properties of

## InS/GaTe heterojunction based on first principles

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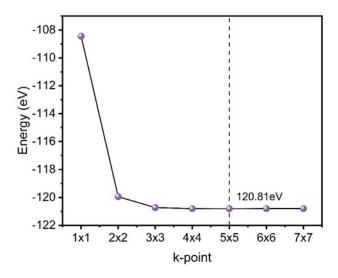


Fig.S1 shows the convergence test of a k-point selection of heterostructure.

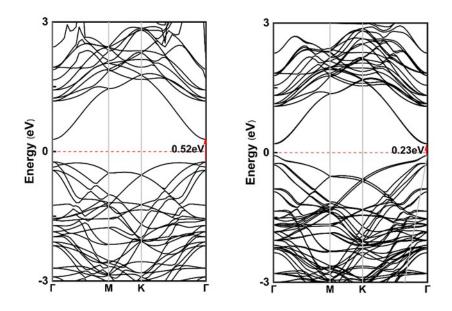


Fig. S2 Band structure of InS/GaTe heterojunction with the (a) projected energy band diagrams and (b) spin-orbit coupling calculated