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Supporting Information

Versatile Two-dimensional Silicon Diphosphide (SiP_2) for Photocatalytic Water Splitting

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Computational details for BSE calculation

For the optical property calculations, NBANDS=160, is used, and the plane-wave energy cut-off was set to 100eV. And the numbers of occupied and virtual bands for electron-hole treatment were set to 8 each.

The electrostatic vacuum potential obtained from HSE06 functional is given below. The value of 3.49 eV is used to shift the CBM and VBM values w.r.t vacuum and to compare with water redox potentials.

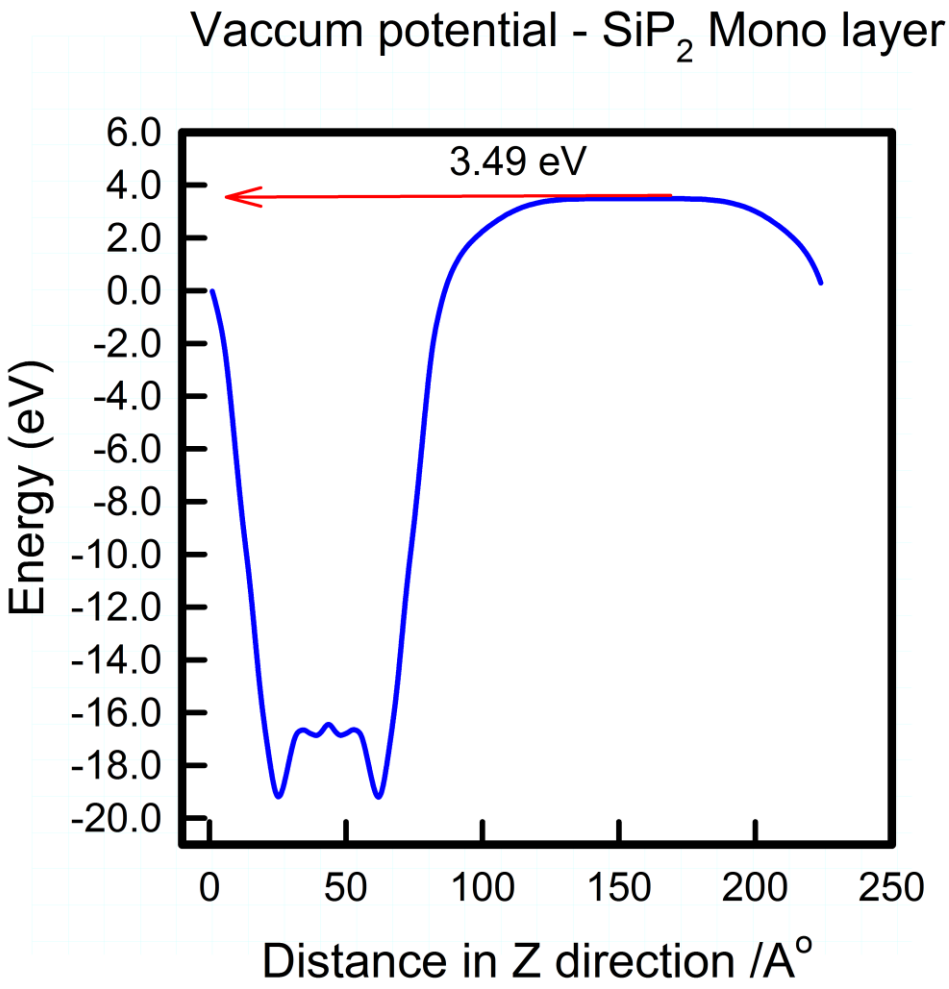

Figure S1 Electrostatic Vacuum potential for SiP_2 monolayer

We studied the PBE functional band gap variation w.r.t tensile strain, it can be seen that the band gap variation is dependent on the direction of lattice. External strain on semiconductor nanostructures would impact electronic properties and thereby optical properties[1, 2].

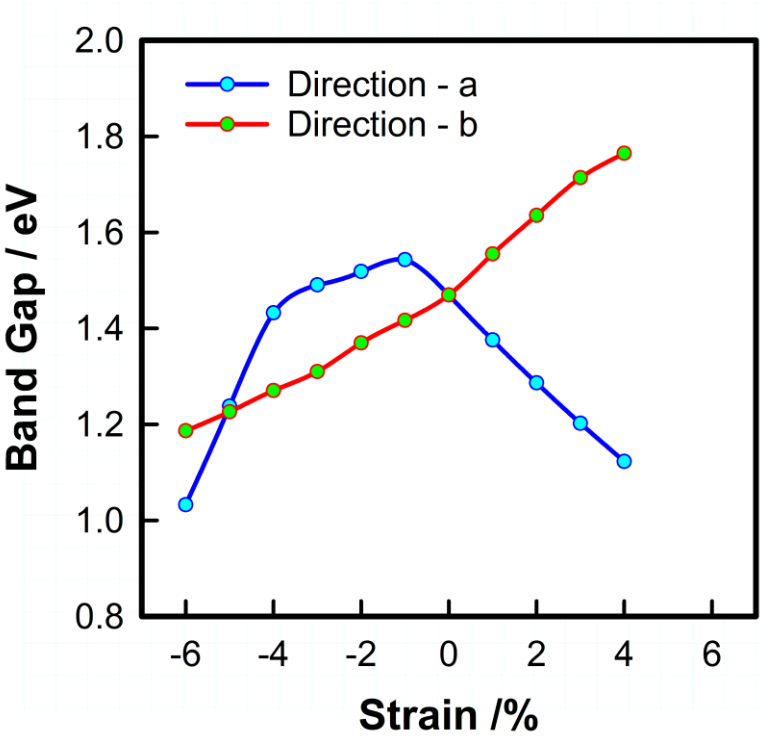

Figure S2 Band gap as a function of biaxial strain calculated with the PBE functional for SiP_2 monolayer

For the calculated absorbance spectrum, it can be seen clearly that the SiP_2 starts absorbing light at about 2.5 eV using GW+RPA method.

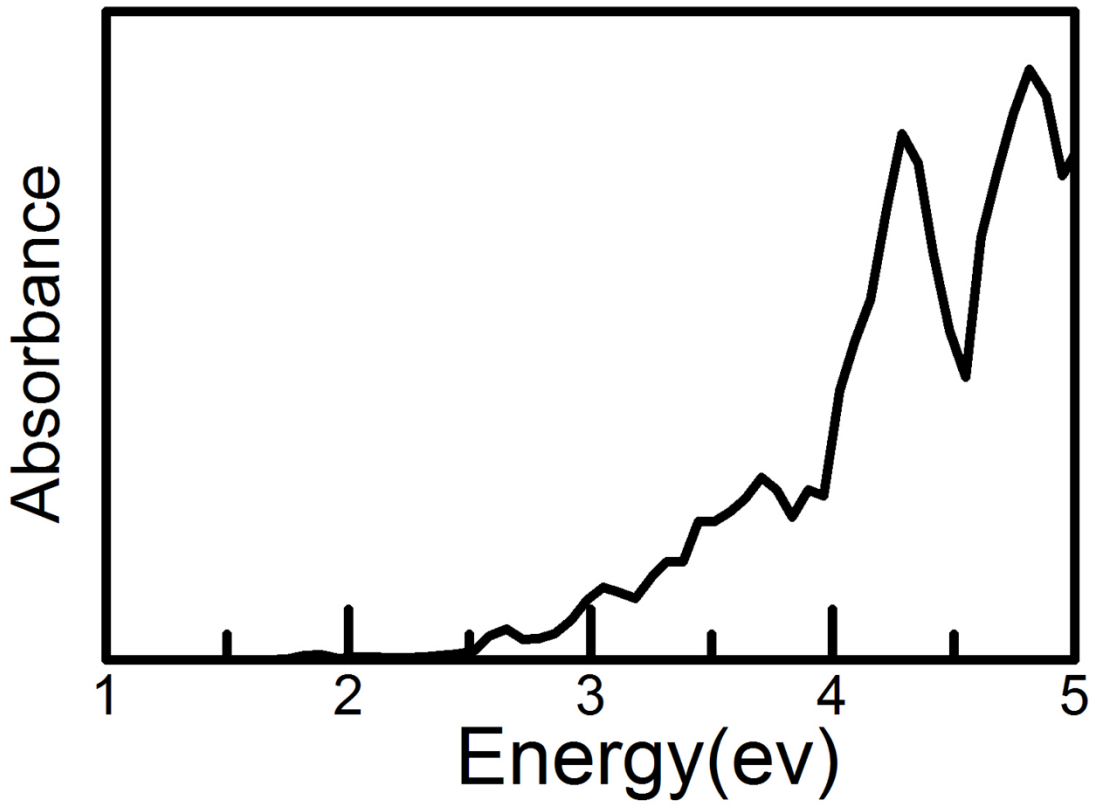

Figure S3 GW+RPA optical absorbance spectrum for 2D SiP_2.

References

1. M. Zhou, W. Duan, Y. Chen and A. Du, *Nanoscale*, 2015, **7**, 15168-15174.
2. F. Ma, M. Zhou, Y. Jiao, G. Gao, Y. Gu, A. Bilic, Z. Chen and A. Du, *Scientific Reports*, 2015, **5**.

