Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Quantum Coupled Borophene Based Heterolayers for Excitonic and Molecular Sensing Applications

Kavita Vishwakarma[1,2], Shivani Rani[1], Sumit Chahal[1], Chia-Yen Lu[3], Soumya Jyoti Ray[1],

Chan-Shan Yang[3,4,*], and Prashant Kumar[1,5,*]

[1]Department of Physics, Indian Institute of Technology Patna, Bihta Campus, Patna-801106, India.

[2]Department of Electronics and Communication Engineering, Indian Institute of Technology Roorkee, Roorkee-247667, India.

[3]Institute and Undergraduate Program of Electro-Optical Engineering, National Taiwan Normal University, Taipei 11677, Taiwan.

[4]Micro/Nano Device Inspection and Research Center, National Taiwan Normal University, Taipei 106, Taiwan.

[5]Global Innovation Centre for Advanced Nanomaterials, The University of Newcastle, University Drive, Newcastle-2308, NSW, Australia.

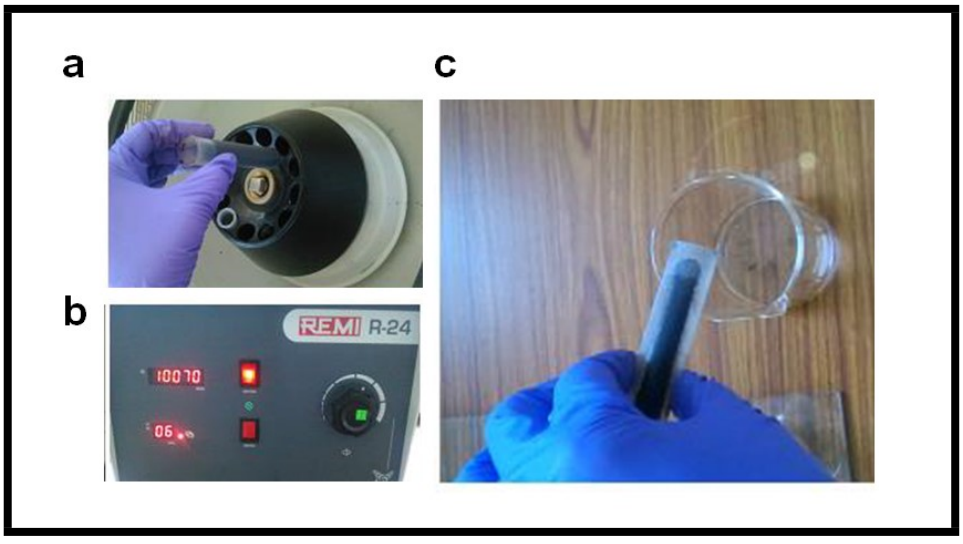

Fig S1. (a, b, c) Camera photograph of different steps of centrifugation.

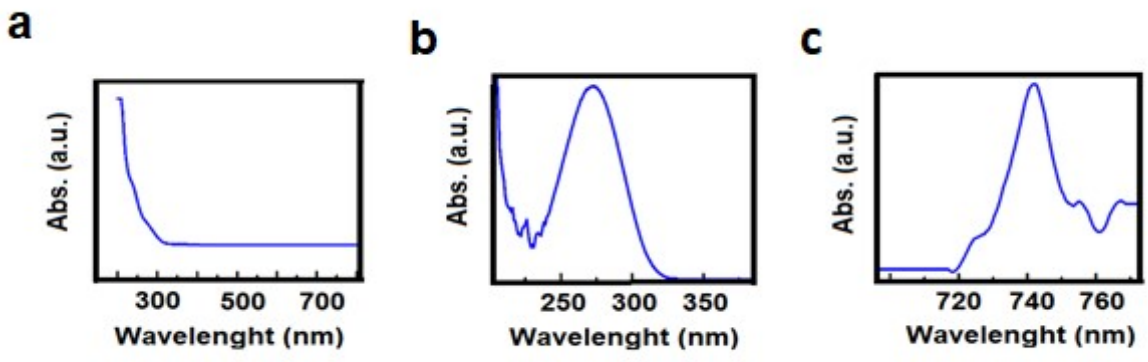

Fig S2. UV-Visible absorption spectra obtained for (a) Borophene, (b) BN and (c) MoS_2.

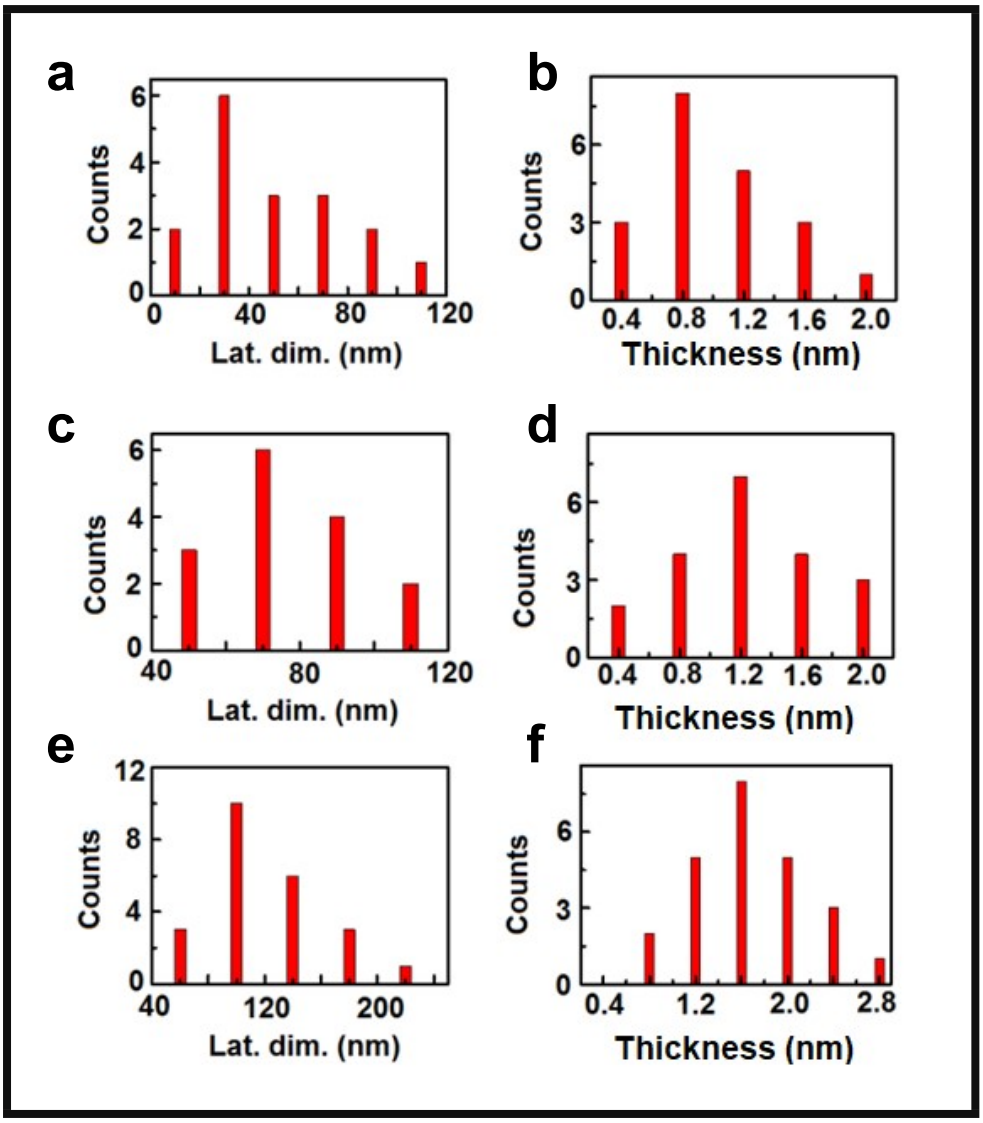

Fig S3. Histograms depicting distribution of lateral dimensions and no. of layers for sonochemically synthesized (a, b) borophene, (c, d) BN and (e, f) MoS_2.

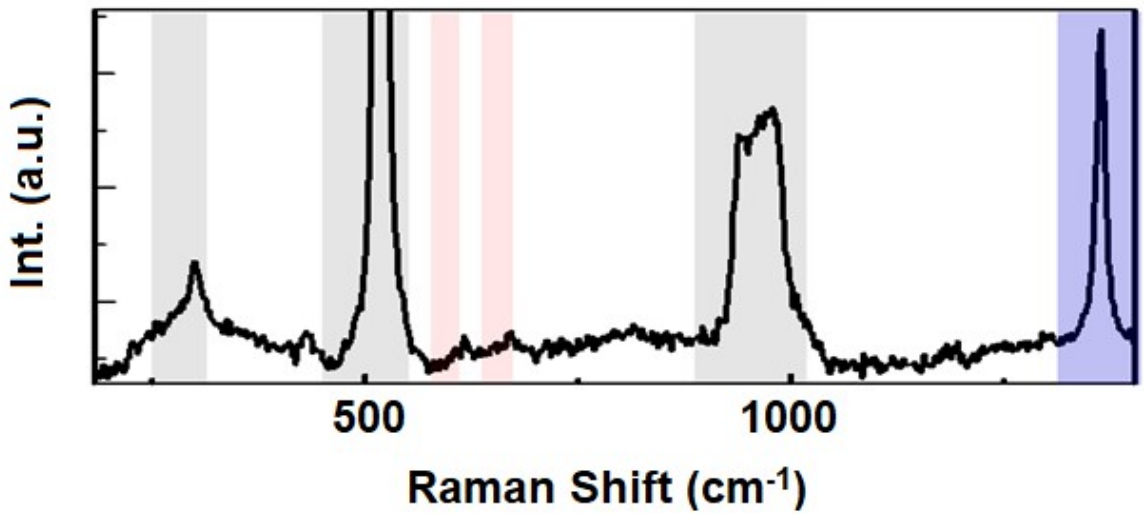

Fig S4. Raman spectrum acquired for heterolayer B/BN.

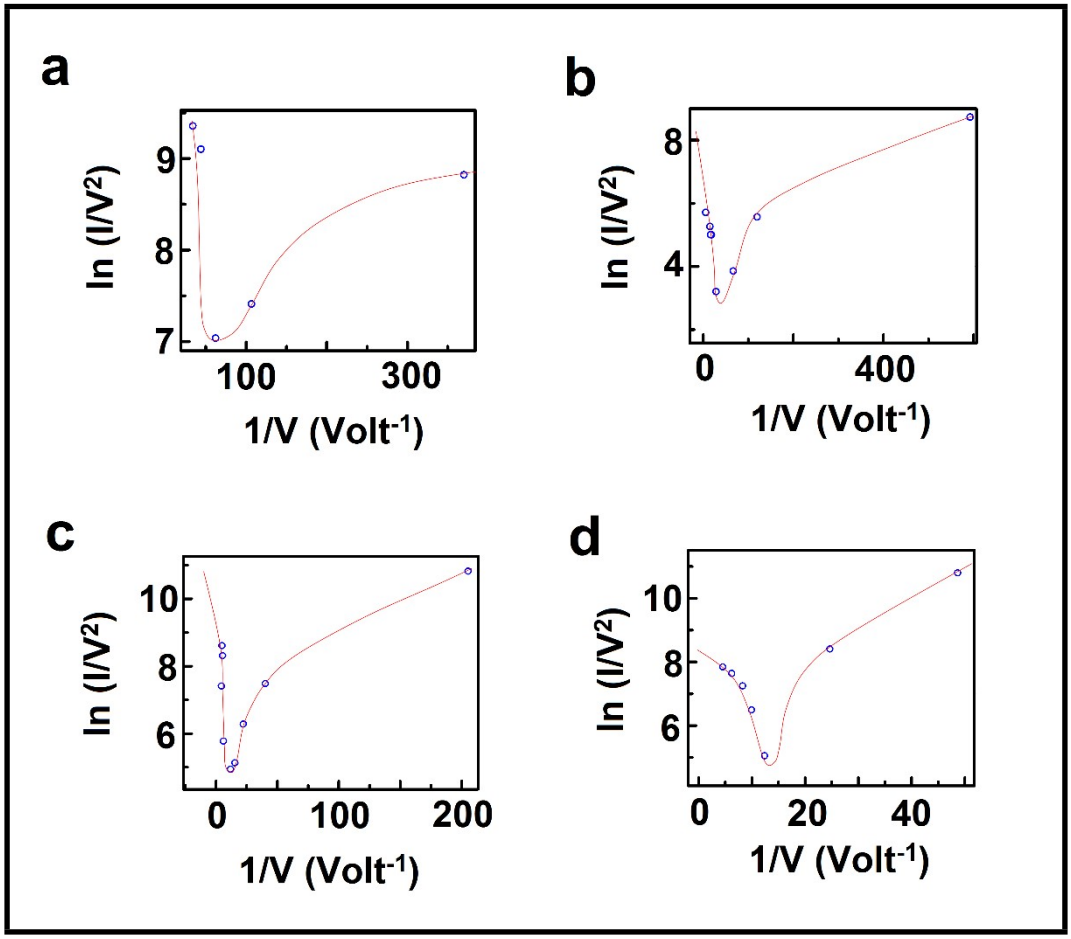

Fig S5. Fowler-Nordheim plot corresponding to CAFM signal for (a) B/BN, (b) B/MoS2 and STM signal for (c) B/BN and (d) B/MoS_2.

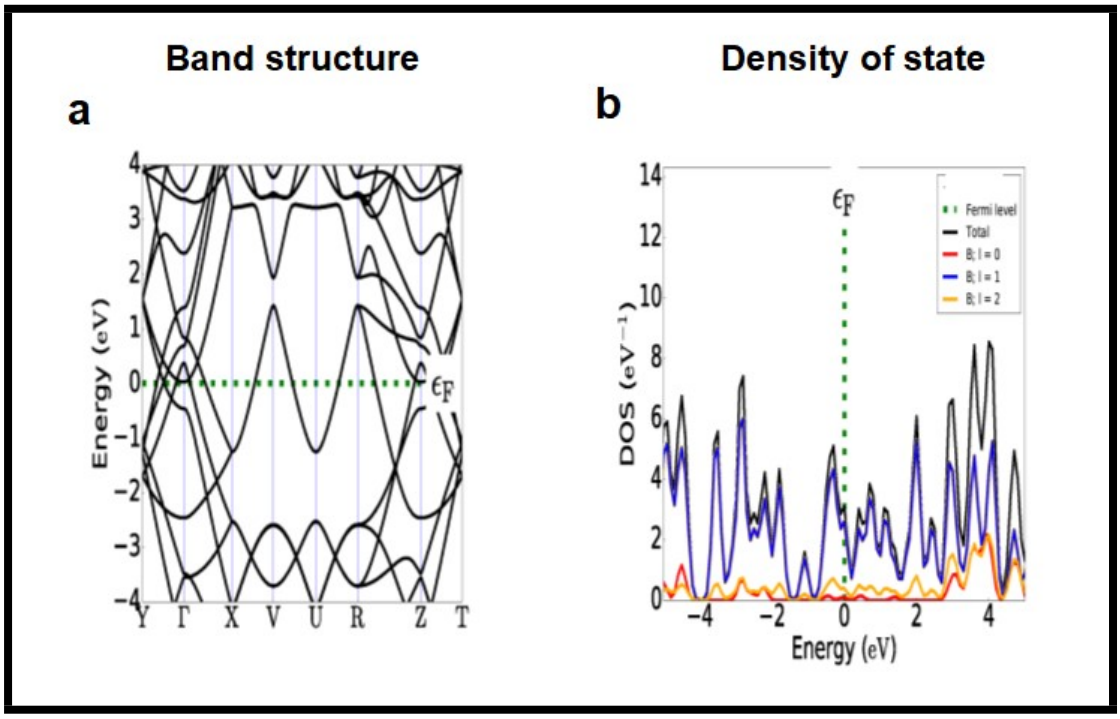

Fig S6. (a) DFT Band structure and (b) density of states (DOS) calculated for monolayer borophene.

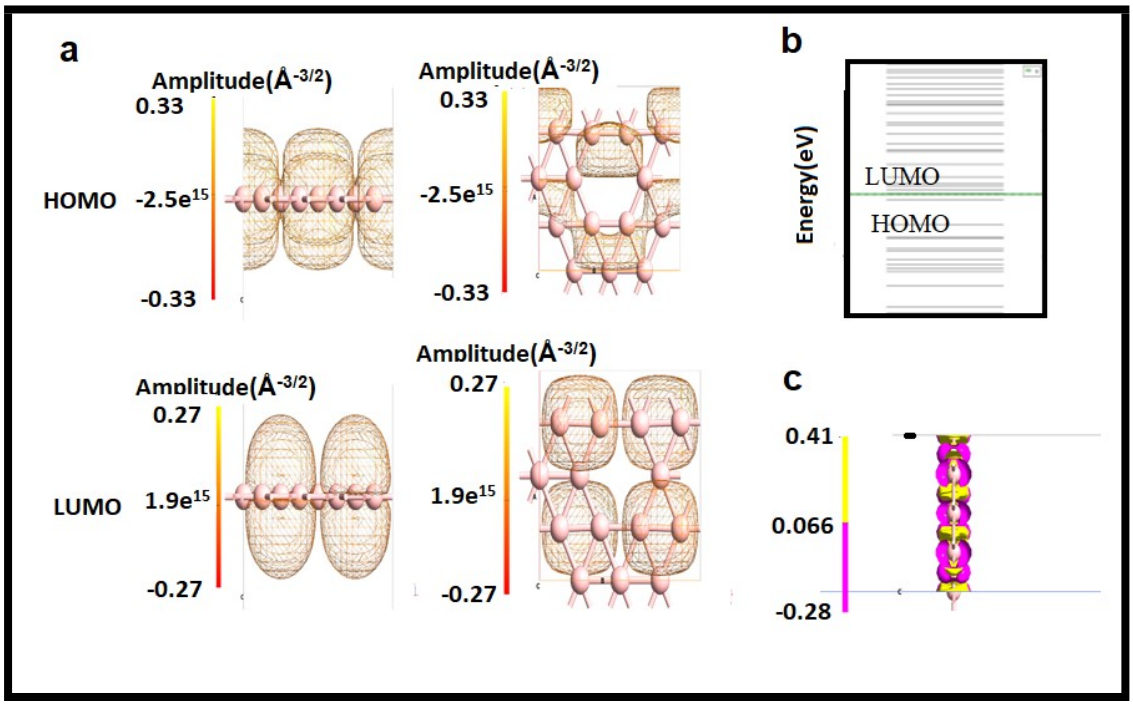

Fig S7. Schematic diagram of (a) side view and (b) top view for HOMO orbital profile and (d) side view, (e) top view for LUMO orbital profile. (c) LUMO/HOMO energy diagram and (f) charge density difference profile of borophene.

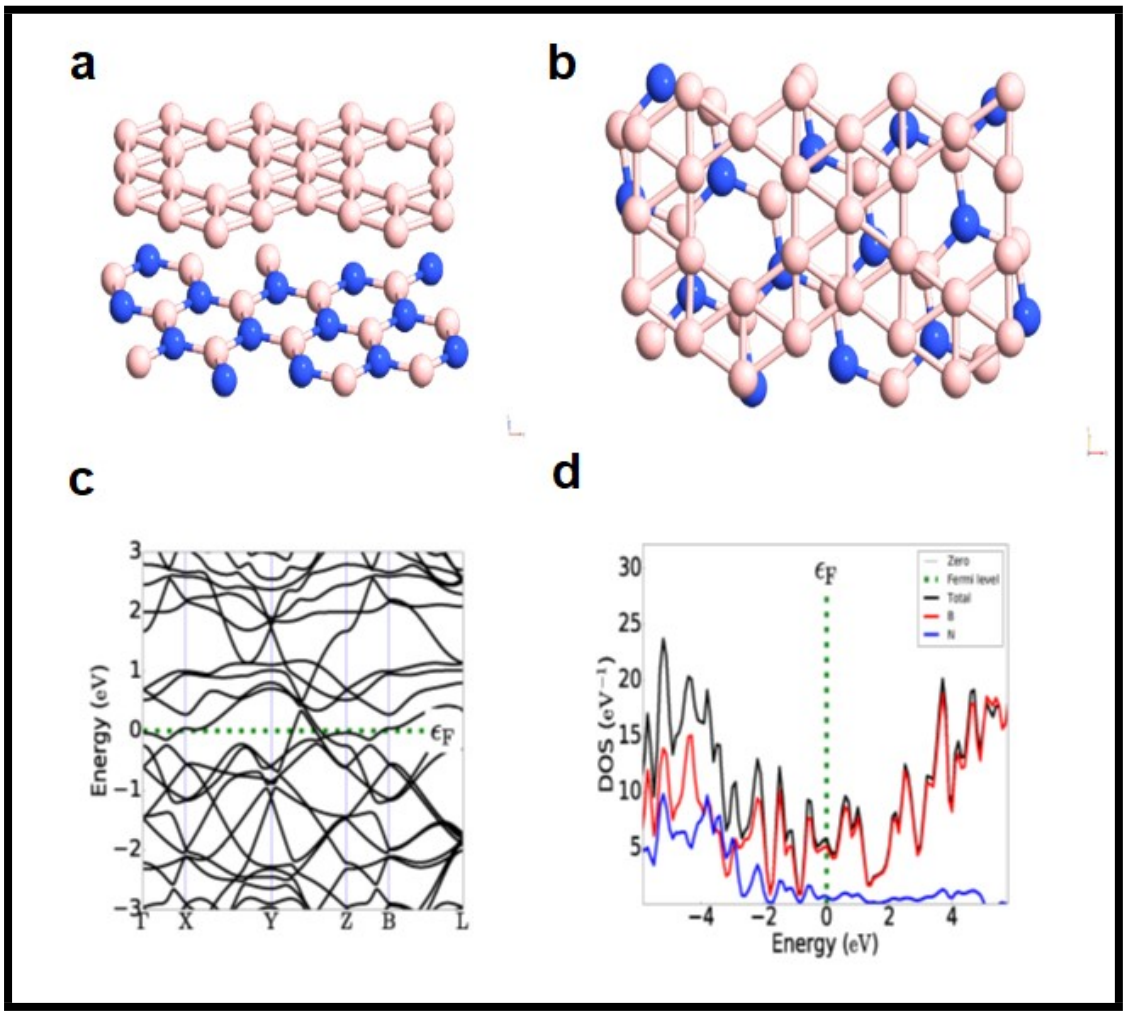

Fig S8. Schematic diagram (a) side view and (b) top view of B/BN heterolayer. (c) DFT band structure and (d) density of states (DOS) calculated for B/BN heterolayer at inter-layer distance 2.5 Å.

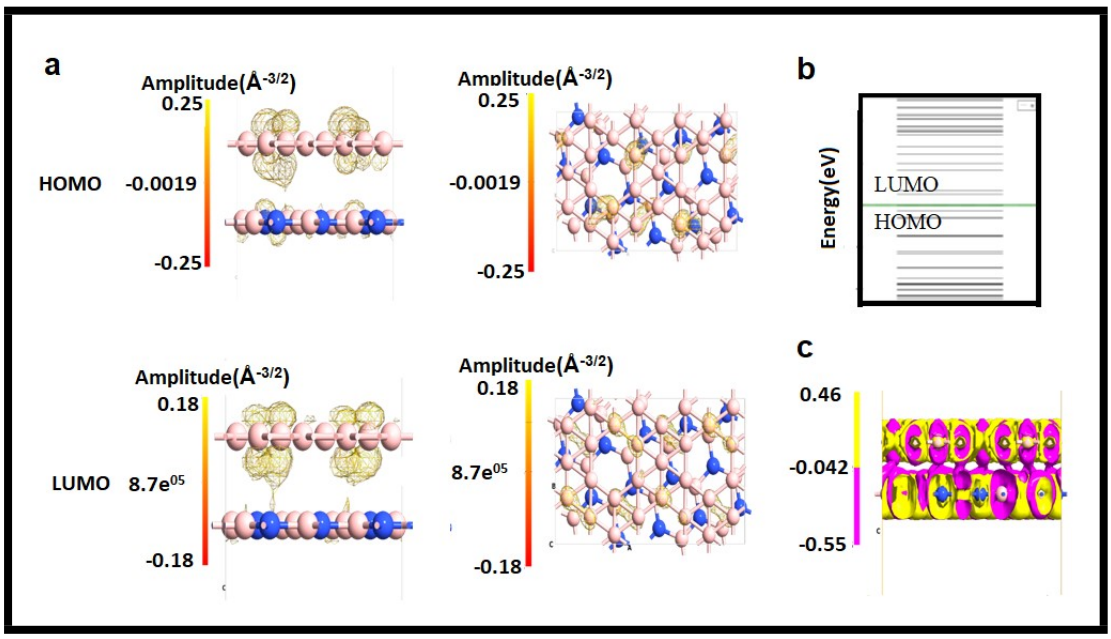

Fig S9. Schematic diagram of (a) side view and (b) top view for HOMO orbital profile and (d) side view, (e) top view for LUMO orbital profile. (c) LUMO/HOMO energy diagram and (f) charge density difference profile of B/BN heterolayer at inter-layer distance 2.5 Å.

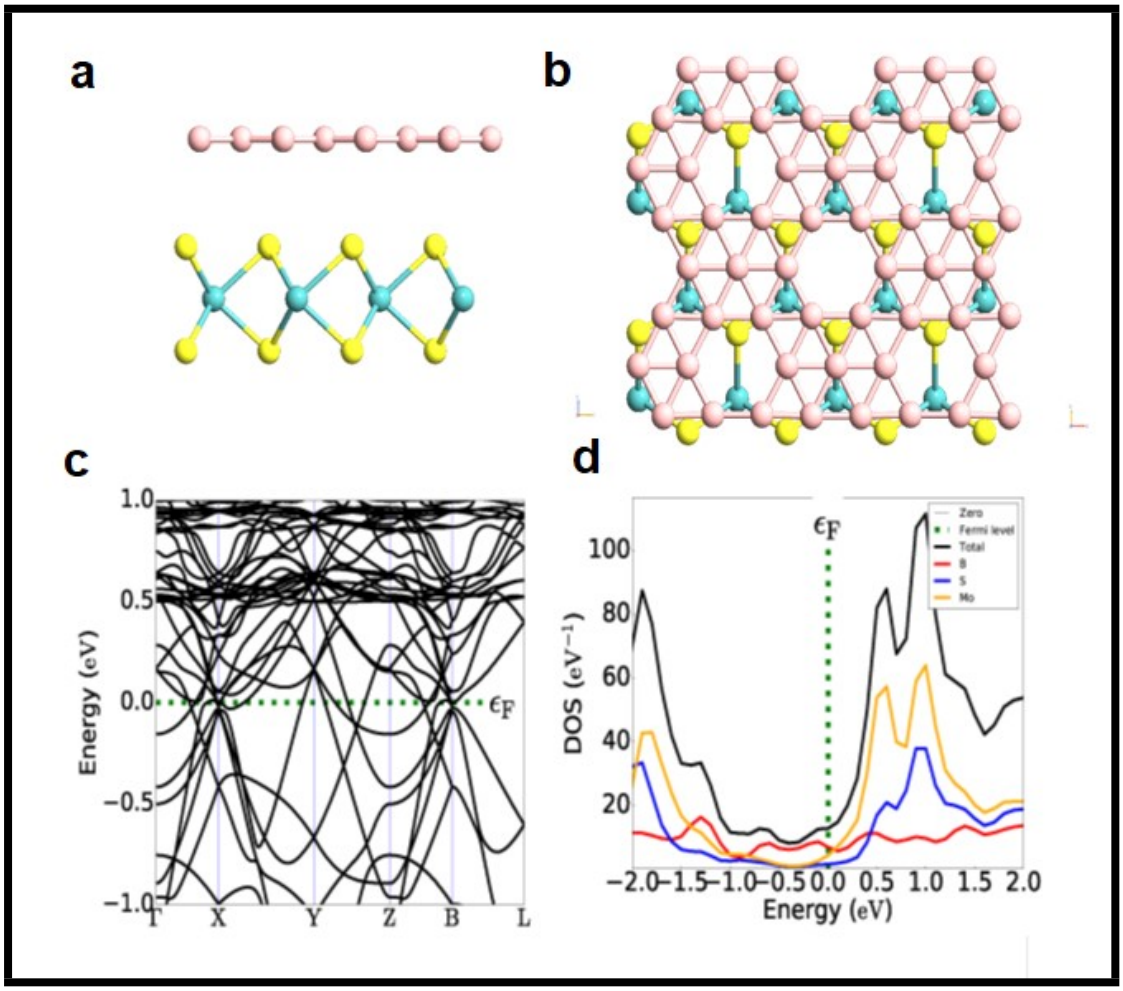

Fig S10. Schematic diagram (a) side view and (b) top view of B/MoS_2 heterolayer. (c) DFT band structure and (d) density of states (DOS) calculated for B/MoS_2 heterolayer at inter-layer distance 2.5 Å.

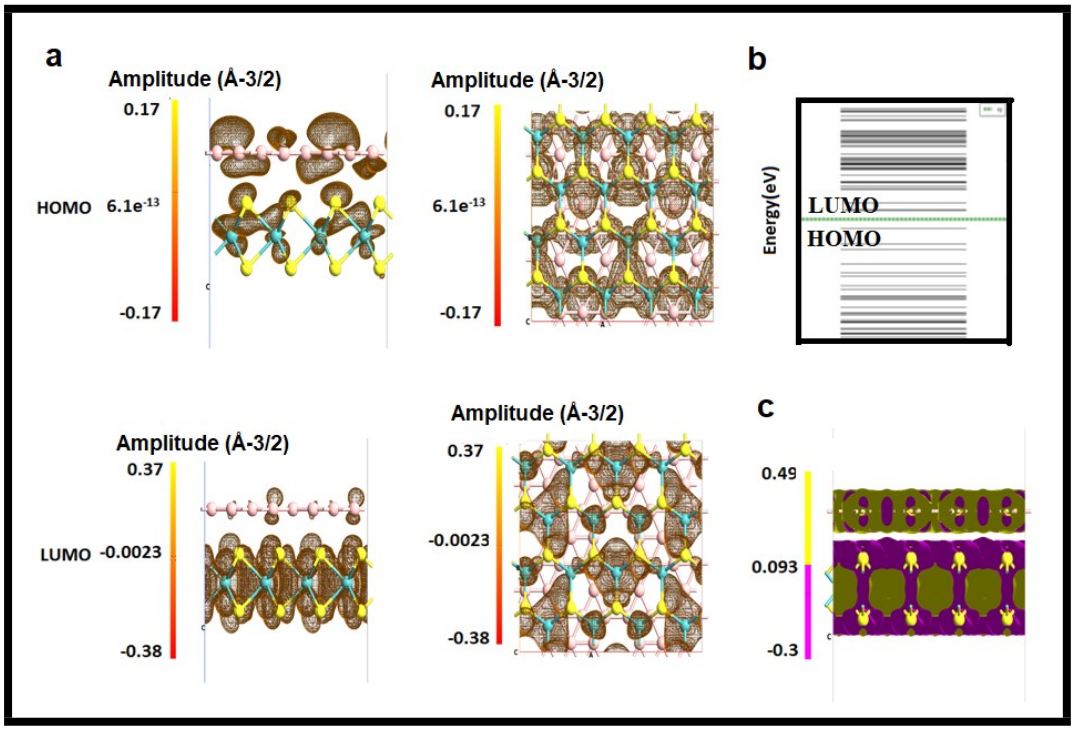

Fig S11. Schematic diagram of (a) side view and (b) top view for HOMO orbital profile and (d) side view, (e) top view for LUMO orbital profile. (c) LUMO/HOMO energy diagram and (f) charge density difference profile of B/MoS_2 heterolayer at inter-layer distance 2.5 Å.

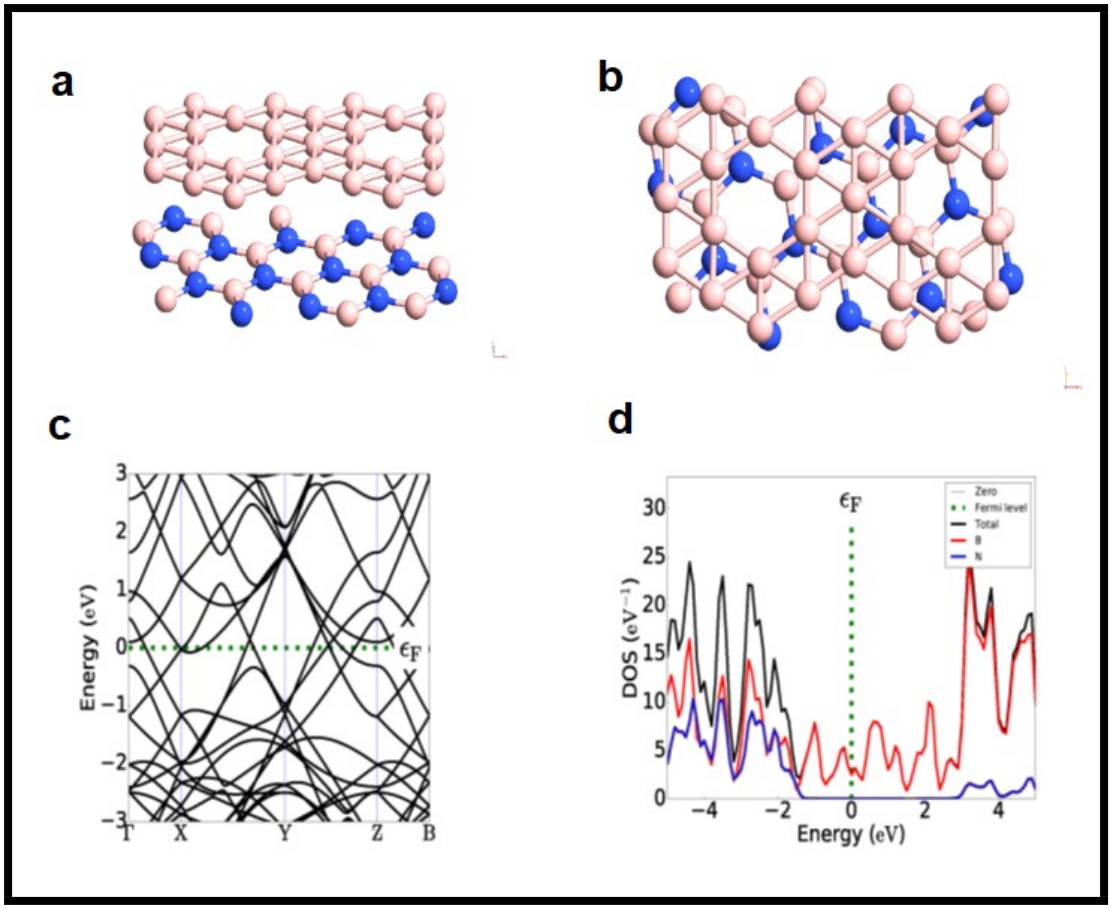

Fig S12. Schematic diagram (a) side view and (b) top view of B/BN heterolayer. (c) DFT band structure and (d) density of states (DOS) calculated for B/BN heterolayer at inter-layer distance 3.77 Å.

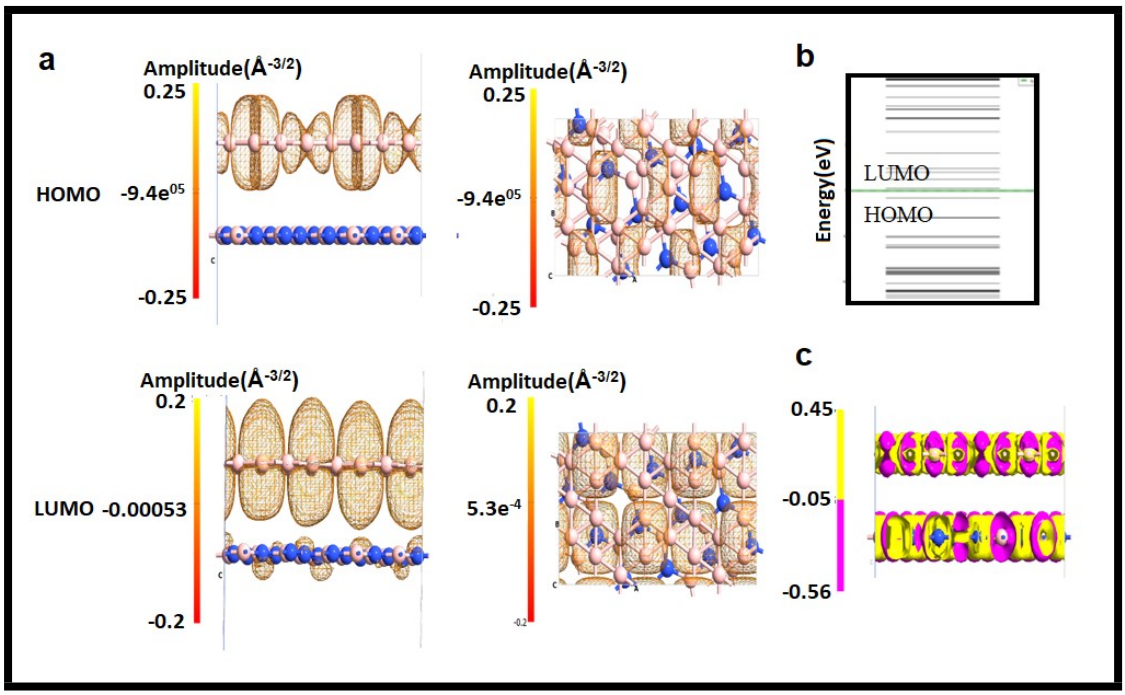

Fig S13. Schematic diagram of (a) side view and (b) top view for HOMO orbital profile and (d) side view, (e) top view for LUMO orbital profile. (c) LUMO/HOMO energy diagram and (f) charge density difference profile of B/BN heterolayer at inter-layer distance 3.77 Å.

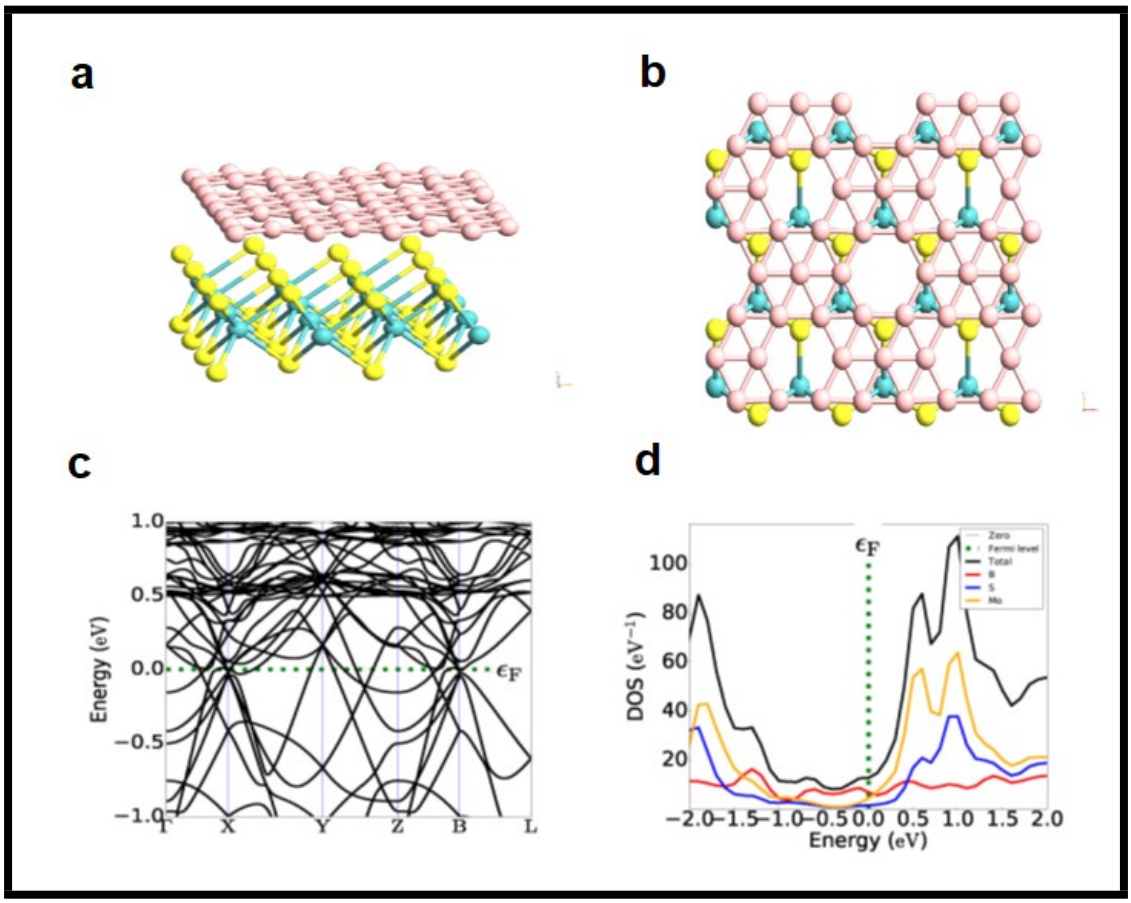

Fig S14. Schematic diagram (a) side view and (b) top view of B/MoS_2 heterolayer. (c) DFT band structure and (d) density of states (DOS) calculated for B/MoS_2 heterolayer at inter-layer distance 3.28 Å.

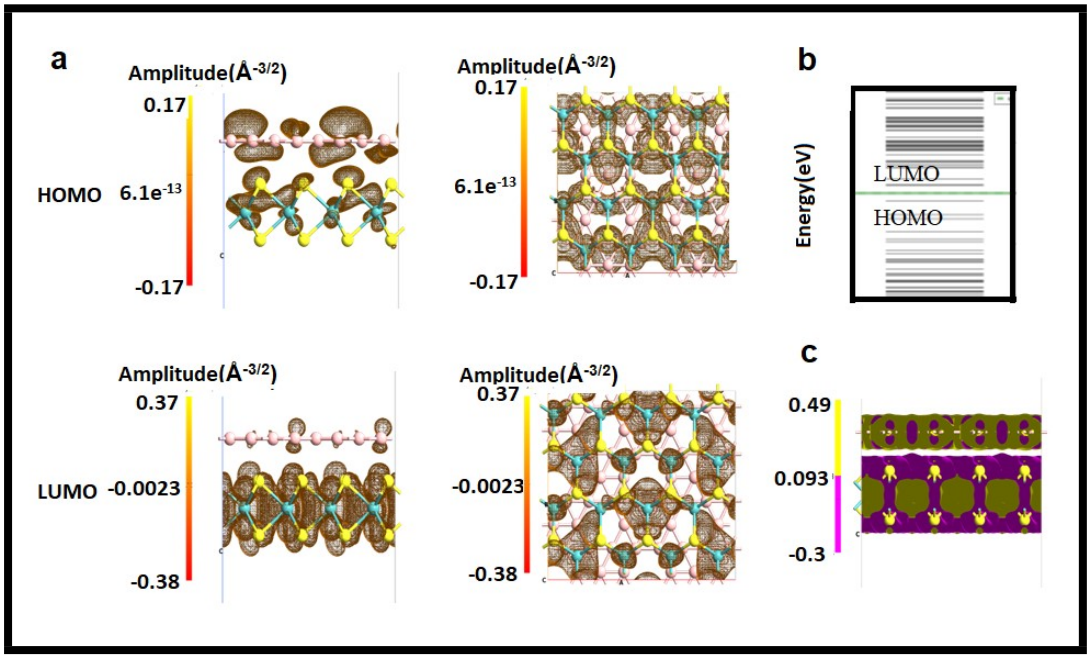

Fig S15. Schematic diagram of (a) side view and (b) top view for HOMO orbital profile and (d) side view, (e) top view for LUMO orbital profile. (c) LUMO/HOMO energy diagram and (f) charge density difference profile of B/MoS_2 heterolayer at inter-layer distance 3.28 Å.