

# Graphene-BC Series Bilayers

## Projected electronic density of state

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## 1. Monolayers

- 1.1 BC<sub>3</sub> (PBE)
- 1.2 Borophene (PBE)
- 1.3 B<sub>4</sub>C<sub>3</sub> (PBE)
- 1.4 Graphene (PBE)

## 2. Bilayers

- 2.1 Graphene-BC<sub>3</sub>: Hollow (PBE)
- 2.2 Graphene-Borophene: Top (PBE)
- 2.3 Graphene-B<sub>4</sub>C<sub>3</sub>: Top (PBE)

# Monolayers: BC<sub>3</sub> (PBE)

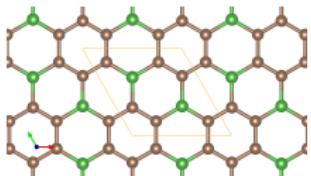


Figure 1: BC<sub>3</sub> supercell

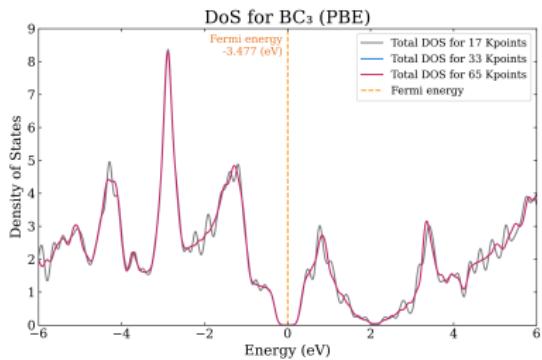


Figure 2: BC<sub>3</sub> DoS

## Monolayer: BC<sub>3</sub>

LUMO band: -3.157700;  
HOMO band: -3.791800;  
Band gap: 0.634100.

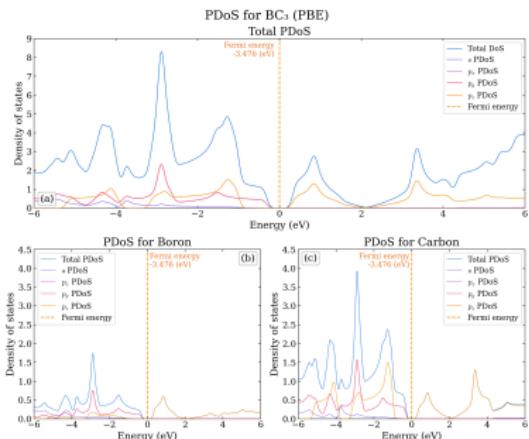


Figure 3: BC<sub>3</sub> PDoS

# Monolayers: Borophene (PBE)

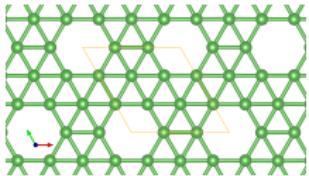


Figure 4: Borophene supercell

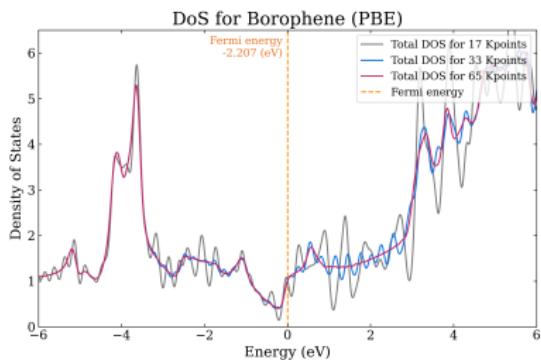


Figure 5: Borophene DoS

**Monolayer: Borophene**  
LUMO band: -2.286900;  
HOMO band: -1.730100;  
Band gap: -0.556800.

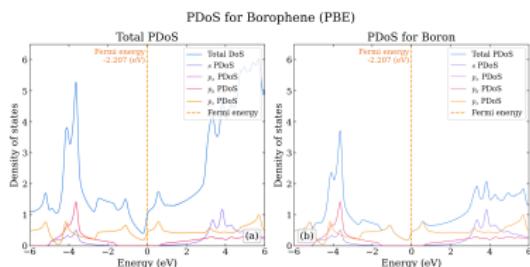


Figure 6: Borophene PDOS

# Monolayers: $B_4C_3$ (PBE)

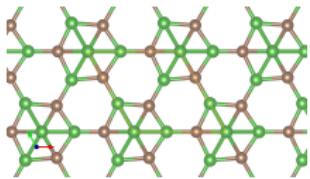


Figure 7:  $B_4C_3$  supercell

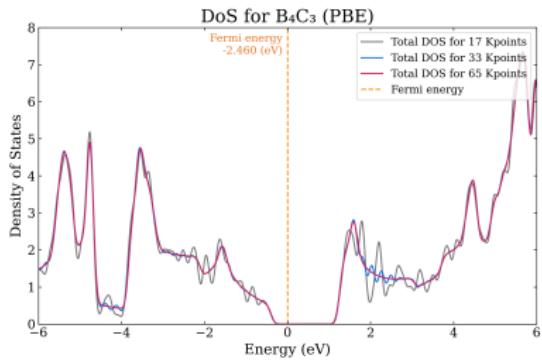


Figure 8:  $B_4C_3$  DoS

## Monolayer: $B_4C_3$

LUMO band: -1.209400;  
HOMO band: -2.855900;  
Band gap: 1.646500.

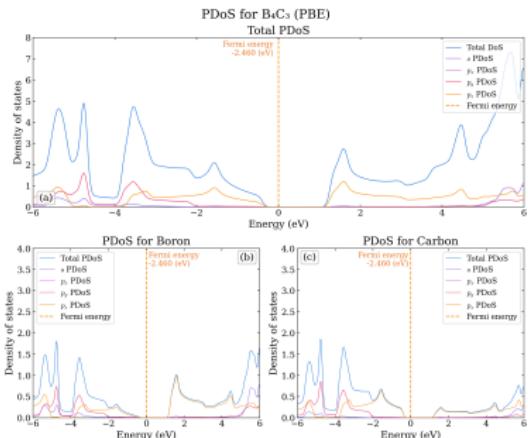


Figure 9:  $B_4C_3$  PDoS

## Monolayers: Graphene (PBE)

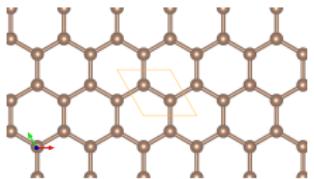


Figure 10: Graphene supercell

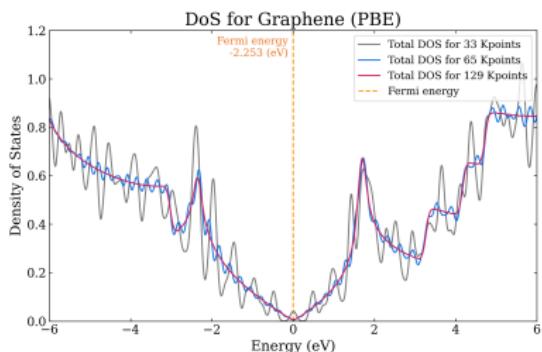


Figure 11: Graphene DoS

**Monolayer: Graphene**  
LUMO band: -2.243900;  
HOMO band: -2.262400;  
Band gap: 0.018500.

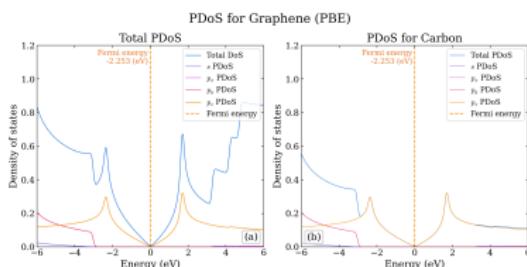


Figure 12: Graphene PDOS

# Bilayers: Graphene- $\text{BC}_3$ : Hollow (PBE)

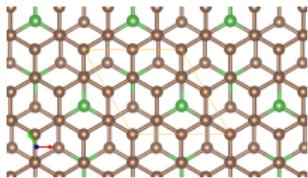


Figure 13: Graphene- $\text{BC}_3$  supercell

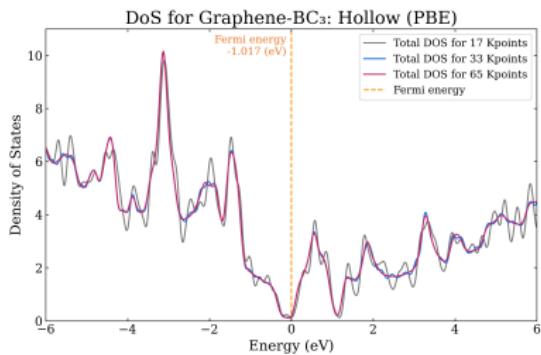


Figure 14: Graphene- $\text{BC}_3$  DoS

## Bilayer: Graphene- $\text{BC}_3$

LUMO band: -0.925600;  
HOMO band: -0.928400;  
Band gap: 0.002800.

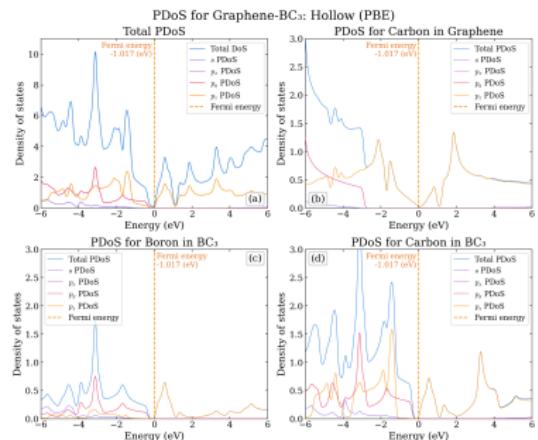


Figure 15: Graphene- $\text{BC}_3$  PDOS

# Bilayers: Graphene-Borophene: Top (PBE)

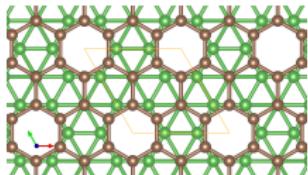


Figure 16: Graphene-Borophene supercell

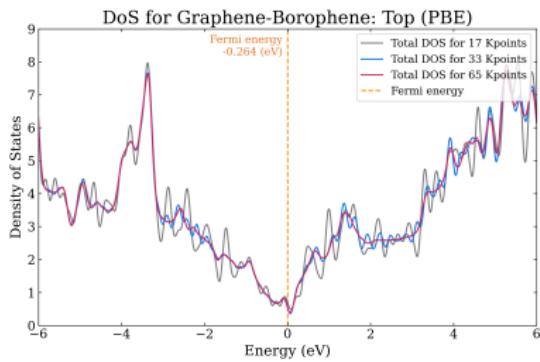


Figure 17: Graphene-Borophene DoS

## Bilayer: Graphene-Borophene

LUMO band: -0.511000;  
HOMO band: -0.310900;  
Band gap: -0.200100.

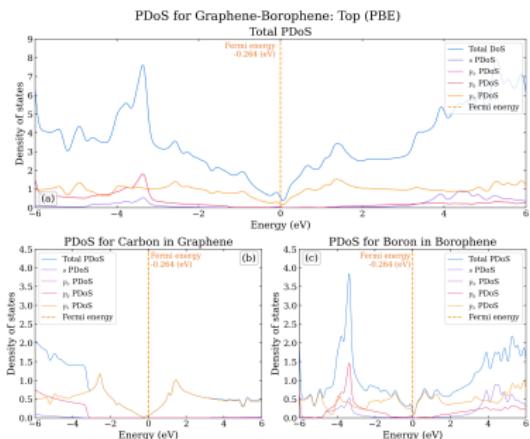


Figure 18: Graphene-Borophene PDOS

## Bilayers: Graphene-B<sub>4</sub>C<sub>3</sub>: Top (PBE)

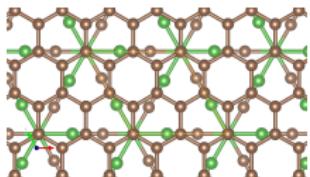


Figure 19: Graphene-B<sub>4</sub>C<sub>3</sub> supercell

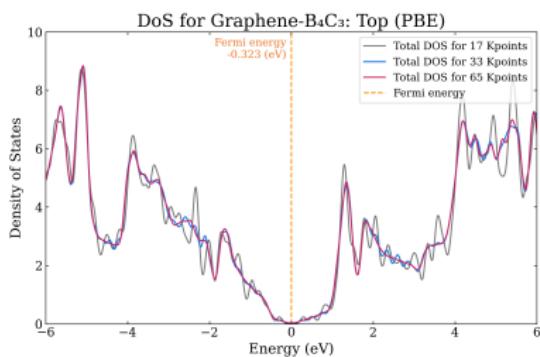


Figure 20: Graphene-B<sub>4</sub>C<sub>3</sub> DoS

## Bilayer: Graphene-B<sub>4</sub>C<sub>3</sub>

LUMO band: -0.314600;

HOMO band: -0.331300;

Band gap: 0.016700.

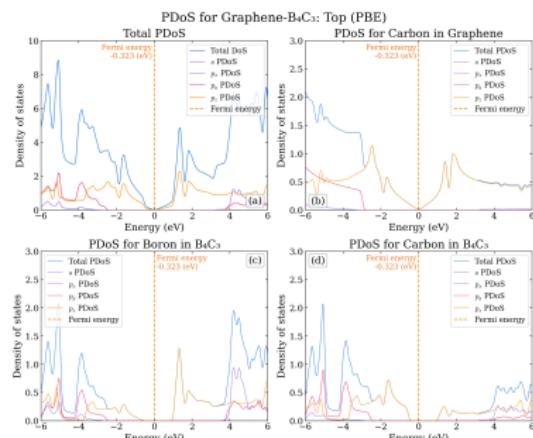


Figure 21: Graphene-B<sub>4</sub>C<sub>3</sub> PDoS

# Thank you