Title:

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Abstract:

Introduction:

Calculation Method:

Results and Discussion:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| System | Lattice Constant | C-C | B-C | B-B | Band-gap (eV) | Nature (direct/indirect) |
| Graphene |  |  |  |  |  |  |
| BC3 |  |  |  |  |  |  |
| B4C3 |  |  |  |  |  |  |
| Borophene |  |  |  |  |  |  |

Top view of these 4 structures like below in Fig. 1. Put the corresponding Band structures, PDOS, phonons, in the SI.



Below give information for favourable structures in a Table, put results for all tested lateral structures in SI, including band structures etc.

Display the dielectric function and absorption coefficient for these 4 structures in Fig. 2 and 3. Here they can be presented like e.g “Outstanding strength, optical characteristics and thermal conductivity of graphene-like BC2 and BC6N”, Carbon, 149 (2019), 733 (absorption up to 20 eV).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Bi-layer  System | Lattice Constant | Strain in Graphene | Strain in BC3/B4C3/B | Interplanar  distance | Band-gap (eV) | Nature (direct/indirect) |
| Graphene-BC3 |  |  |  |  |  |  |
| Graphene-B4C3 |  |  |  |  |  |  |
| Graphene-Borophene |  |  |  |  |  |  |

Give top view of favourable bilayer structures in Fig. 4. Put top views of all atomic structures of all considered bilayer systems in the SI. Put the Energy, vertical distance vs lattice constant plots in the SI.

In Figs. 5, 6, 7 Present band structure, PDOS, and phonon dispersion curves for each of the 3 favourable bilayer system like below.

Dispersion curves

In the SI, but the band structures and PDOS for the other tested bilayer systems.

In Figs. 8, show for the favourable bilayer systems the electron density difference plots in (a), (b), (c).

In Fig. 9, show the dielectric function for the three bilayer systems in (a), (b), (c)



In Fig. 10, show the absorption for the three bilayer systems in (a), (b), (c) (nice to compare to constituent results like in the below).



Having obtained a general understanding of these materials at the GGA-PBE+D3 level, we now investigate if/how the optical properties change using the HSE06.

First show the HSE06 bilayer bandstructures in Fig. 11.

Then in Figs. 12, 13 the dielectric function (a), (b), (c) and the Absorption (a), (b), (c) obtained using HSE06.

Discuss/compare with other systems/results …

For HSE06 I would be happy to do it all at fixed GGA-PBE atomic structures for the sake of time, and expect the lowest energy structures should be the same with PBE and HSE.

If you like, you can check one relaxed bilayer structure with HSE to see.

Conclusion: