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Modification of the bandoffset in boronitrene

Wednesday, 13 July 2011 12:00 (15 minutes)

<p>We carried out ab initio self-consistent calculations to study the modification of the band offsets by polar layers. We considered a double line of C in a monolayer of hexagonal BN, also known as Boronitrene. This effectively introduces a line of dipoles at the interface. We considered BN/C zigzag and armchair configurations. The BN/C zigzag-short is found to be energetically most stable and with the smallest (1.51eV). We show that a two dimensional diode can be constructed from this structure, with changes to the electronic and optical properties of the host system.

Level (Hons, MSc,
   PhD, other)?

PhD

Consider for a student
   award (Yes / No)?

Yes

Would you like to <br> submit a short paper <br> for the Conference
 Proceedings (Yes / No)?

No

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