Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Info

The electronic properties and band-gap discontinuities at cubic boron nitride/diamond hetero-interface

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As it was difficult to obtain a suitable model according to the results of bond length, the band gap of different models were also calculated. The band structures are plotted along high symmetry *K*-points as shown in Fig. S1. As is shown, the band gap of the (111) hetero-structures are direct band gaps, while as to the (100) hetero-structures, the band gaps came to be indirect band gaps. Table S1 reveals the variety of band gaps at (111) hetero-interface. The value of band gap reduce until the slab of BN up to 12 for the C-N bond models. While for the C-B bond ,the value converge completely in the 14 layer model. The result is consistent with the condition which the result of band length expected. In general, shorter bond length means that it has tightly bound atoms, which would lead to higher band gaps. The variety between 12 and 14 layers models were relatively small and the 12 layers model had a better periodicity for calculation and analysis. The value of the direct band gap have a relative deviation compared with the common which often occurs in the DFT calculation. Nevertheless, the 12 *c*-BN-layers models were used in the following calculations to compare with the models of (111) hetero-interface.

Table S1. The calculation results of band gaps at (111) *c*-BN/diamond interface with C-B and C-N bonding configurations.

Interface-bonding	6	8	10	12	14	16
C-B	2.55	2.52	2.49	2.47	2.46	2.46
C-N	2.40	2.37	2.34	2.32	2.32	2.32

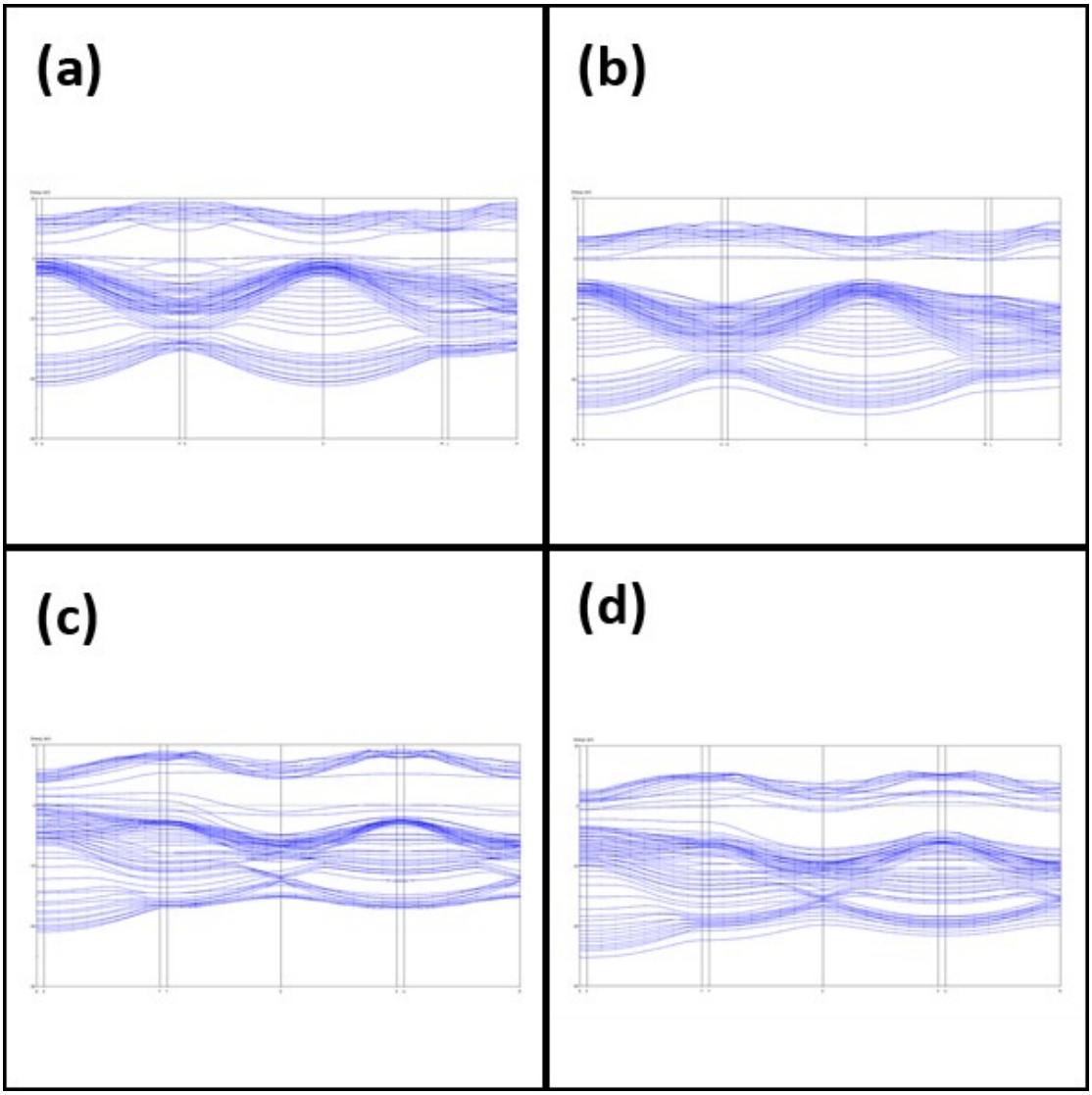

Fig. S1 The band structures of (111) *c*-BN/diamond (a) and (100) *c*-BN/diamond (b) hetero-structures with C-B bonding configuration, (111) *c*-BN/diamond (c) and (100) *c*-BN/diamond (d) hetero-structures with C-N bonding configuration. a and b reveal the direct band gap. c and d show the indirect band gap.