Interaction between Boron Nitride and H-terminated (111) Diamond Surface: A First Principles Investigation

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With the aim of better understanding recent experimental results [1] on field effect transistors (FETs), we performed density functional theory (DFT) calculations on hydrogen-terminated (111) diamond surface with hexagonal boron nitride (BN). In our work, atomic structures and electronic properties of the nanostructures of BN on the hydrogen-terminated (111) diamond surface will be addressed using first-principles DFT based simulation code CONQUEST. The small lattice mismatch of about 0.5% between BN and the H-terminated (111) diamond surface is predicted in good agreement with previous experiments [2,3]. The binding energies of the various stacking patterns, the density of states, and the charge density distribution [see Fig.1] are calculated and analyzed. It turns out that weak van der Waals interactions dominate for BN on these H-terminated (111) diamond surface. Our results provide a better understanding of the interfacial properties of BN/H-diamond and pave the way to further design field effect transistors (FETs) having high mobility and high carrier density in nanoelectronics.

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References:

1. T. Yamaguchi and co-workers, *APL Materials* **6**, 111105 (2018).
2. R. Reeber and K. Wang, *J. Electron. Mater*. **25**, 63 (1996).
3. W. Paszkowicz, J. B. Pelka, M. Knapp, T. Szyszko, and S. Podsiadlo, *Appl. Phys. A* **75**, 431 (2002).

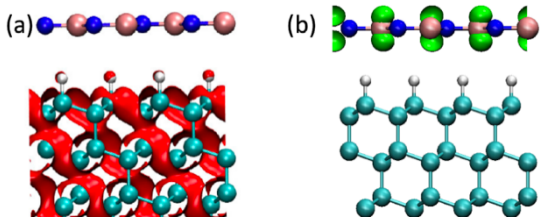

Fig.1: Real space charge density distribution of (a) valence band maximum and (b) conduction band minimum for the BN/H-diamond heterostructure.