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Study On Electronic Properties And Bonding Configuration At BN/SiC Interface

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The electronic properties and bonding configuration at the interface between cubic (zinc blende) BN and 3C-SiC are studied using the first principle linear muffin-tin orbital (LMTO) method based on local-density-functional (LDA) theory. The (001) superlattice of BN(n)/SiC(n) (n=1-5) is used to study the interface. The calculated results show that the preferred bonding configuration is Si-N and C-B for the (001) BN/SiC interface. The formation energy of the interface is studied as a function of thickness of the superlattice. The origin of the bond formation as well as the electronic properties of the interface are also investigated.