We calculated the electronic and lattice properties of 5H-BN. 5H-BN is an sp³ bonded compound as wurtzite BN (2H-BN) and cubic BN (3C-BN). This is a hexagonal layered structure which is determined uniquely. The lattice properties were optimized automatically by the first-principles molecular dynamics (FPMD) method. The calculated lattice properties agree well with experimental results[1][2]. A calculated electronic band structure of 5H-BN is non-metallic and its band gap is indirect. Valence band maximum (VBM) and conduction band minimum (CBM) of 5H-BN is \( \Gamma - L \).