First-principles study of 5H-BN

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We calculated the electronic and lattice properties of 5H-BN. 5H-BN is an sp^3 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 Γ - *L*.

[1] S. Komatsu, K. Okada, Y. Shimizu and Y. Moriyoshi, J. Phys. Chem. B **103** (1999) 3289.
[2] S. Komatsu, A. Okudo, D. Kazami, D. Golberg, Y. Li, Y. Moriyoshi, M. Shiratani and K. Okada, J. Phys. Chem. B **108** (2004) 5182.