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Spontaneous phase transition of nano-sized boron nitride – A quantum size effect[1] HONGLI DANG, University of Tulsa, Y.G. SHEN, City University of Hong Kong, SANWU WANG, University of Tulsa — We report first-principles quantum-mechanical calculations that predict a novel phase transition of nano-sized boron nitride (BN) thin-films. When the thickness of the BN thin-film is below 1.4 nm, a spontaneous phase transition from the diamond-like structure to a graphite phase is predicted. The process would involve no energy barriers. When the thickness of BN increases, on the other hand, energy barriers for the phase transition would appear and gradually increase with the thickness. Calculations show that while the graphite structure has a lower total energy than the corresponding diamond-like structure for the BN thin-film with any thickness, the spontaneous phase transition would occur only when the size is small. We attribute this phenomenon to the quantum size effect.

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