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Thermal Properties of Carbon Doped Monolayer h-BN Systems: A Tight Binding Model Study

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Abstract: We report here a tight binding model study of hexagonal boron nitride (h-BN) 50% doped with carbon (C) atoms at the boron or nitrogen sublattice sites. The model Hamiltonian is written considering the effect of first, second and third nearest neighbor hopping interactions. The model Hamiltonian is solved using Zubarev's Green's function technique to find out the electron density of states. The temperature dependent entropy and specific heat for pure h-BN, h-BC and h-CN systems are computed and compared.

Keywords: Hexagonal boron-nitride; electron/hole doping; specific heat

[Full Paper]