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Band dispersion of monolayer insulating Boron Nitride: A minimal tight-binding model study

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Abstract. We report here a tight-binding minimal model for single layer boron nitride (s-BN) taking into account of the site energy of boron and nitrogen atoms along with electron hopping parameters into third nearest neighbors. The electronic Green's functions are calculated by using Zubarev's Green's function technique. Finally the band dispersions for s-BN are computed numerically and plotted for different tight-binding parameters to give a wide band gap of $E_g = 5.01eV$

Keywords. Band dispersion, monolayer h-BN

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[Full Paper]