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Electronic and field emission properties of BN/C nanotubes

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BN/C nanotube superlattices are quasi one-dimensional heterostructures that show unique physical properties, due to the ionicity of the B-N bond and the low symmetry of their structures. Using state-of-the-art first-principles calculations, we have investigated their electronic and field emission properties. First, we show how BN/C systems can be used for effective band offset nanodevice engineering. The band-offset flexibility occurs because the band gap of the BN nanotube section is largely symmetry-independent, while that of the carbon section is highly sensitive to the diameter and helicity. The polarization of the BN section, present in all BN nanotubes except the armchair ones, can introduce a strong macroscopic electric field in the superlattice, despite the screening due to the carbon section. The intrinsic electric field induces substantial changes in the work function at the tip of the BN/C system. This effect can vastly improve the field emission properties, since the decrease in the work function exponentially increases the current density, compared to a pure carbon nanotube.

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