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Band Gap Renormalization in Semiconducting Carbon Nanotubes NICHOLAS LANZILLO, NEERAV KHARCHE, SAROJ NAYAK, Rensselaer Polytechnic Institute — We use first-principles density functional theory (DFT) in conjunction with the GW Approximation to show that the presence of a dielectric substrate is found to alter the electronic properties of semiconducting carbon nanotubes. In particular, a substrate-induced polarization effect stabilizes the correlation energy in both the valence band maximum and the conduction band minimum, resulting in a decrease in the electronic band gap. This effect is due to non-local dielectric screening which can be described accurately through the GW Approximation but is not captured in DFT alone. While similar band gap renormalization effects have been observed for isolated molecules and even for two-dimensional materials on substrates, this is the first prediction of such an effect in a strictly one-dimensional geometry. We find that the magnitude of the band gap reduction is on the order of 0.5 eV when deposited on a hexagonal boron nitride substrate. This type of band gap modulation is of great importance in developing future opto-electronic devices.

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