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Quasi-particle Energy Gap of Metal-coated Carbon Nanotubes
YU ZHOU, LI CHEN, YIMING ZHANG, SWASTIK KAR, PULICKEL AJAYAN, SAROJ NAYAK, Rensselaer Polytechnic Institute — We have studied the electronic structures of metal-coated carbon nanotubes using density functional theory and many body corrections based on GW approximation (GWA). In particular, we will present energy band gap variation as a function of number of metal atoms on the nanotube surface. Our results are compared with recent experiments.

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