Assembling Low Dimensional Material Composites for Applications in Photonics

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The integration of select low dimensional materials like graphene, graphitic carbon nitride, phosphorene, and noble metal nano clusters for the formation of composite assemblies via noncovalent interactions are investigated using first principal Density Functional Theory (DFT) studies. Different interaction sites of these low dimensional counterparts are probed to promote assemblies that consist of selected material couples from the aforementioned list. These assemblies are capable of displaying unique optical and electronic properties that could be further tuned by monomer modification techniques like functionalization and dimensionality control. Band gaps, absorption/plasmonic response, emission/luminescence properties, electron hole distributions, charge carrier recombination lifetimes, shifts in density of states, and charge transfer at material boundaries are investigated for all assemblies and their viability for different applications in the field of photonics is assessed. Furthermore, we look at how probing the non-covalent interactions that hold these materials together via selective tuning of the donor accepter sites by functionalization affect the composite properties.