

Architecturing Graphene Interfaces and Functionalized Nanoparticles for Nanotechnology and Bionanoscience

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Interesting structural and electronic effects are observed when electronically or chemically doped graphene is interfaced with metal surfaces or molecular layers. In the first part of this talk we review some examples that have been simulated in our group by means of density functional theory (DFT) calculations and compared with experimental results: N-doped graphene interfaced with Ni(111) [1,2,3], B-doped graphene interfaced with Ir(111) [4], Fe-doped graphene interfaced with Pt(111) [5], and p-type doped graphene interfaced with a nickel-phthalocyanine (NiPc) monolayer [6] or functionalized with tetrazine [7].

The second part of the talk is devoted to functionalized transition metal oxide nanoparticles (i.e. TiO₂ and Fe₃O₄) for biomedical applications. Atomic models of realistic size (2-4 nm, i.e. 800-4000 atoms) are used to simulate, at a quantum mechanical level of theory in combination with classical molecular dynamics, the structural, electronic and magnetic properties of these nanosystems, their interaction with light and with the aqueous environment. Surface functionalization with stabilizing polymers or functionalizing molecular species for drug delivery, targeting and imaging is also investigated [8-11].

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