Interfacing doped graphene with metal surfaces or molecular layers.

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

References

[1] "Inside out" growth method for high-quality nitrogen-doped Graphene. Carbon 171 (2021) 704e710

[2] "Spatial segregation of substitutional B atoms in graphene patterned by the moiré superlattice on Ir(111)" Carbon 201 (2023) 881–890

[3] in preparation

[4] "π-Orbital mediated charge transfer channels in a monolayer Gr–NiPc heterointerface unveiled by soft X-ray electron spectroscopies and DFT calculations" Nanoscale 14 (2022) 13166

[5] "Pushing Down the Limit of NH_3 Detection of Graphene-Based Chemiresistive Sensors through Functionalization by Thermally Activated Tetrazoles Dimerization" ACS Nano 16 (2022) 10456−10469