Non-covalent Interactions to Graphene: Theory and Experiment

Petr Lazar,[a] František Karlický,[a] Jaroslav Granatier,[b] Eva Otyepková,[a] Matúš Dubecký,[a] Radek Zbořil,[a] Pavel Hobza,[a,b] Mingdong Dong,[c] Michal Otyepka[a]

[a]Regional Centre of Advanced Technologies and Materials, Department of Physical Chemistry, Faculty of Science, Palacky University, Olomouc, Czech Republic

[b]Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic

[c]iNANO, Aarhus University, Aarhus, Denmark

Graphene is a two-dimensional π-conjugated material having extraordinary physical properties, which makes its a perspective material in catalysis, energy storage, nano(opto)electronics and sensor applications.[1] The application potential of graphene can be enormously enhanced by its covalent and non-covalent functionalization.[2] An exact quantification of interaction between graphene and guest molecules as well as thorough understanding of the nature of interaction between graphene and guest molecules have not been yet achieved. We analysed nature of interaction between Ag, Au, Pd, Pt metal atoms and clusters to benzene, coronene and graphene, by quantum chemical calculations [3,4] The silver atom is bound weakly by London dispersion forces, while interaction of palladium and platinum is significantly stronger and involves some covalent character. Involvement of relativistic effects is required for a reasonable description of interactions involving Au and Pt. We measured the interaction force between metalized AFM tips (Cu, Ag, Au, Pt and naturally Si were considered, Figure) and graphene and correlated the results with theoretical calculations carried out by density functional theory (DFT). The theoretically calculated interaction forces agree with the experimental data, only when non-local electron correlation and exact Hartree-Fock electron exchange is explicitly treated.[5] The AFM tip covered by copper displayed the highest affinity to graphene among the metals considered. We also quantified the adsorption enthalpies between graphene and several organic molecules and compared the experimental results with theoretical calculations carried out by DFT, SCS(MI)-MP2 and CCSD(T) calculations.[6]

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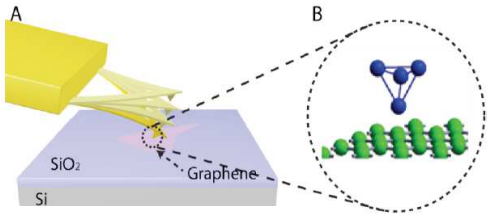

Adopted from Ref. [5].