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Tenkých vrstev a nanostruktur

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TÉMA

Non-covalent Interactions to Graphene: Theory and Experiment

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Graphene is a two-dimensional carbon-based honeycomb lattice having extraordinary physical properties, which makes graphene a perspective material in catalysis, energy storage, nano(opto)electronics and sensor applications.[1,2] The application potential of graphene can be enormously enhanced by its covalent and non-covalent functionalization.[3] However, thorough understanding of the nature and strength 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. [4-6] 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 of Au and Pt. We also measured the interaction force between metallized atomic force microscopy (AFM) tips (Cu, Ag, Au, Pt and naturally Si were considered, Figure 1) by dynamic AFM and graphene under ambient conditions. We correlated the experimental 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.[7] 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 by inverse gas chromatography. Theoretical calculations carried out by DFT, various post Hartree-Fock (including MP2 and CCSD(T)) methods and symmetry adapted perturbation theory (SAPT) computations enabled to decipher the nature of interaction between organic molecules and graphene. The organic molecules are dominantly bound by dispersive London forces. This also explains the fact that only DFT methods accounting for non-local electron correlation effects give adsorption enthalpies in a good agreement with the experiment.[8]

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| [1] | Novoselov KS et al. Science 306, (2004) 666. | [5] | Granatier J et al. J. Phys. Chem. C 116, (2012) 14151. |
| [2] | Novoselov KS et al. Nature 490, (2012) 192. | [6] | Granatier J et al. J. Chem. Theory Comput. 9, (2013) 1461. |
| [3] | Georgakilas V et al. Chem. Rev. 112, (2012) 6156. | [7] | Lazar P et al. ACS Nano 7, (2013) 1646. |
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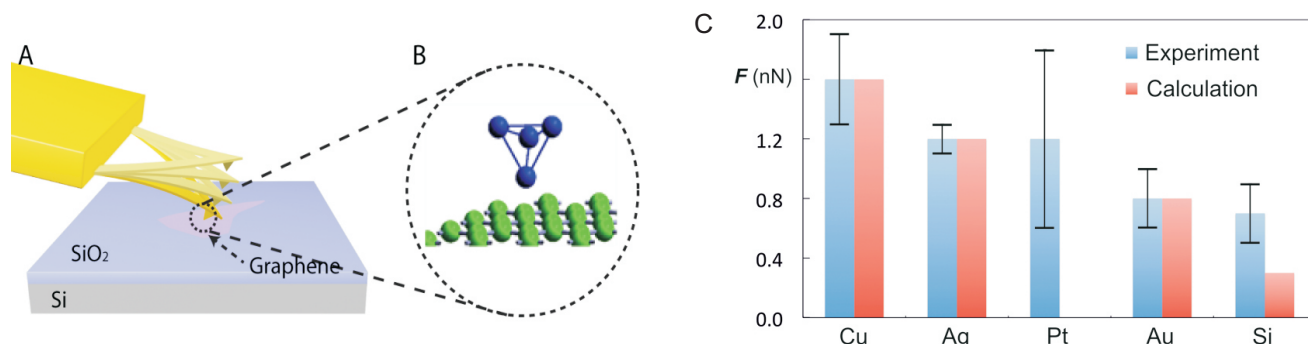


Figure 1 A: The interaction force between graphene and metallized AFM tip was measured by dynamic AFM at ambient conditions. B The model used for theoretical calculations involves graphene (green) and metal tetrahedron (blue). C: Comparison between measured and calculated forces. Adopted from ref [7].

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