Deposition of *N*-Heteropolycycles on Graphene

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In recent years, noncovalent functionalisation of graphene with organic molecules has attracted considerable attention due to the possibility of controlled chemical doping. Graphene shows strong π-π interactions with aromatic molecules allowing the deposition of a range of organic materials from solution with scope for molecular self-assembly[1]. However, a number of aspects have not been sufficiently addressed, For example, it is unclear in which way the periphery around the aromatic core and potentially pre-organisation of the molecules prior to deposition has an impact on supramolecular arrangement and packing density on the surface. In addition, it is particularly difficult to quantitatively relate the doping strength to the donor/acceptor properties of the molecules, as molecular packing (governed by the overall structure of the molecule) has to be decoupled from electronic properties (governed by the aromatic core).

In our study we use different classes of *N*-Heteropolycycles for the noncovalent functionalisation of CVD graphene with the aim of chemical doping. This class of organic molecules is especially suitable, as the structure can be systematically varied. In particular, the donor/acceptor strength can be varied via the substitution pattern of the nitrogen in the core (for example pyridinic N and pyrrolic N) and thus tuned independently from the molecular periperhy.

We focus on derivatives of tri-isopropylsilyl-Tetraazapentacene[2] (TIPS-TAPs) and Tetraazaperopyrene[3] (TAPPs) to investigate i) the effects of different deposition methods (drop-casting, dip-coating from different solvents) ii) various ligands in the periphery of the aromatic core on the supramolecular arrangement on the graphene surface and the impact on chemical doping of the graphene. Raman (in combination with AFM/KPFM) is a particularly versatile characterisation technique, as both doping and packing density of the molecule can be evaluated simultaneously.

References

[1] *Nanoscale* (2015) 7, 16337-16342.
[2] *Angew. Chem. Int. Ed.* (2013) 52, 3810 – 3821.
[3] *Chem. Eur. J.* (2015) 21, 17691.

Figures

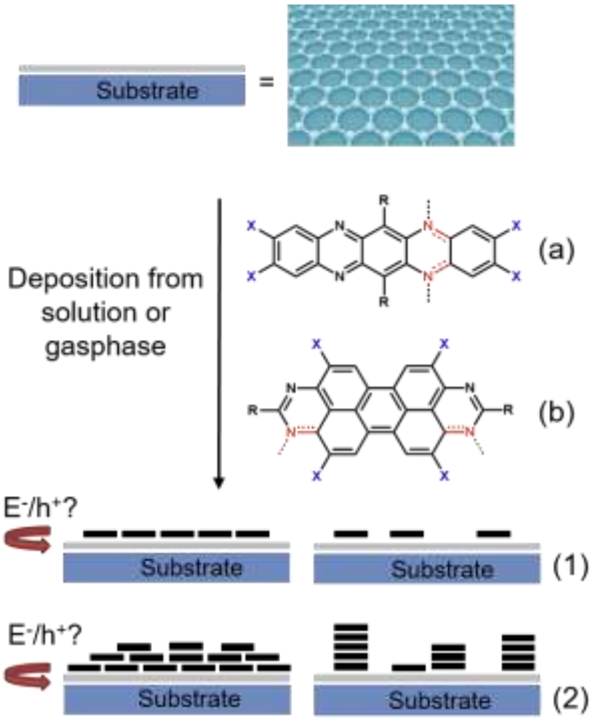

Figure 1: Possible structures of *N*-Heteropolycycles on graphene: flat monolayer (**1**), crystalline stacked (**2**). (**a**) and (**b**) represent the general structure of TAPs and TAPPs respectively. The donor/acceptor strength can be varied independently from the periphery via the structure of the nitrogen in the cor