Physics of *h*-BN and gr mono-layers on metal substrates

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Abstract:
The mono-layer of hexagonal *h*-BN is an interesting material by itself, and further so by complementing the graphene (*gr*) mono-layer realm by being an insulator, whereas the latter carries the well-known semi-metallic character. This allows *h*-BN to be used as a separator of adsorbed species from the support material beneath.

We have recently characterised several structures where *h*-BN has been grown on the surface of a transition or coinage metal. These combined experiment-simulation studies have included supports from Cu(111) to Rh(111) to Ir(111), exposing Moiré patterns, where the *h*-BN becomes either electronically (Cu) or geometrically (Rh, Ir) corrugated at a lateral scale of few nano-metres.

Here we shall present a qualitative study using density functional theory (DFT) simulations of how the *h*-BN mono-layer affects the electronic structure seen by adsorbed atoms or molecules. We pay particular attention to how the electro-static potential is modified, and compare how *h*-BN and *gr* act as separator layers.

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Dehalogenation and coupling of a polycyclic hydrocarbon on an atomically thin insulator, Thomas Dienel, Jaime Gómez-Díaz, Ari Paavo Seitsonen, Roland Widmer, Marcella Iannuzzi, Kevin Radican, Hermann Sachdev, Klaus Müllen, Jürg Hutter and Oliver Gröning, *ACS Nano* **8** (2014) 6571-6579

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Contribution: Invited ☒