Growth of two dimensional *h*-BN: Influence of the support on the electronic and optical properties of the

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1. Growth of hexagonal boron nitride (*h*-BN) of high quality

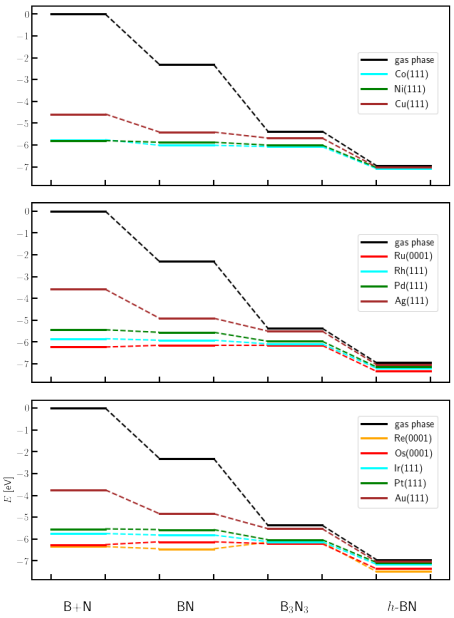

Fig. 1. Energy diagrammes of formation of *h*-BN from single atoms to dimers to hexamers to full mono-layer; from Ref [3]

The single layer of the hexagonal boron nitride (*h*-BN) is an insulator that can be used to separate adsorbed species from the underlying substrate, both physically and electronically. The production of high-quality *h*-BN is essential for the ultimate performance of two dimensional (2D) materials-based devices, since it is the key 2D encapsulation material. We are working on the optimisation of the procedures to grow *h*-BN on surface of transition metals.

Our recent achievements include the enhanced quality of the *h*-BN on Rh(111) via 2D distillation [1], and a decisive guideline for fabricating high-quality *h*-BN on Pt(111) [2]. We have found that it is crucial to exclude carbon from the *h*-BN related process, otherwise carbon prevails over boron and nitrogen due to its larger binding energy, thereupon forming graphene on metals after high-temperature annealing. We introduce the pyrolysis temperature T_p as an important quality indicator for *h*-BN on transition metals.

In order to understand better the underlying physical trends, we have performed systematic density functional theory (DFT) calculations of fragments to the full mono-layer of *h*-BN on 12 different hexagonally oriented transition metals [3]. We further report corresponding studies carried out on graphene. We will also show results from DFT calculations of Moiré structures, where the *h*-BN sheet can be vertically bent.

2. Consequences of adsorption on the electronic and (linear) optical properties of *h*-BN

We are carrying out calculations of the electronic properties of the *h*-BN when supported on the various substrates. Also we report some preliminary results of the influence of the support on the linear optical properties of the *h*-BN. Further we will discuss the properties of adsorbed molecules on the supported *h*-BN that could be used for example as single molecule magnets, such as endo-fullerenes with lanthanide elements adsorbed inside the fullerene cage .

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4. References

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