A monolayer of hexagonal boron nitride on Ir(111) as a template for cluster growth

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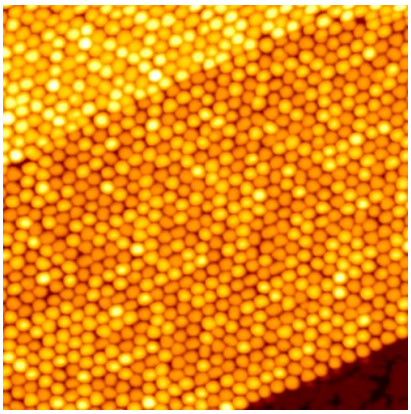
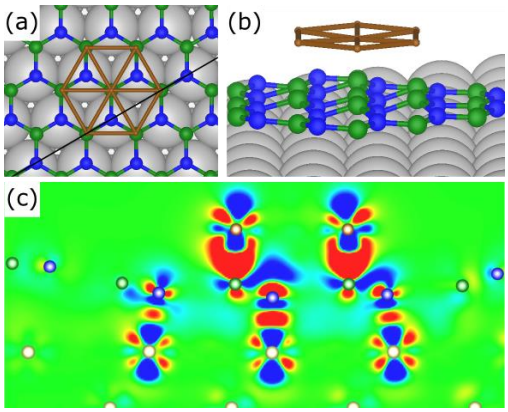
Chemical vapor deposition of borazine molecules on Ir(111) results in a well aligned monolayer of hexagonal boron nitride (h-BN) which forms an incommensurate (11.7 x 11.7) moiré on (10.7 x 10.7) substrate unit cells. The center of each unit cell provides a chemisorbed valley area, where h-BN is hybridized with the Ir substrate [1]. Through a scanning tunneling microscopy study we provide evidence that the valley regions are reactive and pin deposited atoms. As a result, highly regular cluster arrays with a periodicity of 2.9 nm can be formed. For the case of Ir deposition, the size distribution is narrow. The average cluster size can be tuned from a few to about 200 atoms for room temperature deposition. The thermal stability of the clusters is extraordinairy, with a decay of the cluster lattice setting in only above 700 K, through intercalation and Smoluchowski ripening. *Ab initio* calculations explain the remarkably strong Ir cluster binding through selective sp^3 rehybridization of the h-BN sheet, involving a boron-Ir cluster bond and a strengthening of the nitrogen bonds to the Ir substrate in the valley area.

We demonstrate the versatility of the approach and find regular cluster lattice formation also in the case of Au and C deposition at room temperature. Regularly positioned C clusters are even observed after annealing to 1500 K. Compared to cluster lattices using graphene on Ir(111) as a template, the better ordering and the higher thermal stability make the arrays on h-BN/Ir(111) superior for potential applications, *e.g.* in nano-catalysis.



90 nm x 90 nm STM image of 0.57 ML Ir on h-BN on Ir(111) deposited at 250 K and imaged at 300 K



(a) top view of relaxed DFT geometry of an Ir heptamer on h-BN on Ir(111). (b) Perspective side view of the same geometry. (c) Charge difference plot through the black line in (a). Red stands for charge accumulation, blue is charge depletion. N atoms are depicted as blue balls, B atoms are green, Ir substrate atoms are grey, and Ir cluster atoms are brown.

References:
[1] Ferdinand H. Farwick zum Hagen et al., ACS Nano **10.12**, 11012-11026 (2016).