Hexagonal boron nitride on transition metal surfaces: A perspective from density functional theory

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Single layer of hexagonal boron nitride (h-BN) can form both commensurate and incommensurate structures when adsorbed on surfaces of transition and noble metals. The latter form Moire patterns that lead to different vertical corrugation, sometimes up to about 1 A. These have periodities of several nanometres and can act as templates for adsorbed atoms and molecules (http://www.nanomesh.ch/).

In this contribution we shall review our recent calculations [1] using density functional theory (DFT) to support and explain recent experiments on the h-BN structures on Ni(111), Cu(111), Ru(0001) and Rh(111). We make connections to methods which provide information of the geometrical (LEED, STM, SXRD) and electronic (STM, STS, ARPES) structure of these systems.

[1] J Gomez Diaz et alia, *Theoretical Chemistry Accounts* **132**, 1350 (2013).