Moire' structure or nanomesh: the case of graphene and h-BN epitaxially grown on transition metals

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Modern nanotemplates based on hexagonal boron nitride or graphene. are robust and promising substrates for self-assembly, electron confinement or intercalation. The characteristic Moire` superstructures formed by a single layer of boron nitride or carbon on the supporting metal are determined by the mismatch between the lattice constant of the exposed hexagonal surface and the sp2 layer.
Recently we have developed a model for the simulation of this type of structures, which is based on large- scale density functional theory calculations [1-3]. We applied the model to describe the adsorption of boron nitride and graphene on several substrates, being able to reproduce and explain experimental findings. Thanks to the computational efficiency of our simulation algorithms, we can afford systems of several thousands of atoms, thus being able to properly describe the structural and electronic corrugation [4]. We also investigated the adsorption of molecules on such modulated structures, also in this case being of substantial help in the interpretation of experimental observations [5-6].
In this talk, I will also present recent results on the formation and equilibration of defects generated by ion implantation onto the hBN/Rh(111) system. The selectivity of the implantation process is discussed in terms of structural and electronic properties.
In conclusions, we believe that our work is a valuable contribution in the understanding of sp2 hybridized layers on surfaces.
This work is done in collaboration with the group of Prof. T. Greber at the physic institute of the university of Zurich.

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