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Substrate induced modulation of physical and chemical properties of quasi two-dimensional nanostructures

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In the post-Graphene era, several quasi two-dimensional nanostructures have been grown epitaxially on metallic or semiconducting substrates, resulting in heterojunctions with interesting application potential. Physical and chemical properties of such overlayers often get modulated by the sub-surface layers of the corresponding substrates, leading to manifestation of new properties. In this talk, I shall discuss how density functional theory (DFT) based first principles approach can be used for a microscopic understanding of such interface induced effects. Such phenomena depend crucially on the exact geometry of the interface which in turn is self-consistently inter-twinned with its electronic structure. Some case studies will be discussed viz. (a) Silicene monolayers on III-V and II-VI semiconducting substrates : undergo n-type (p-type) doping on metal/nonmetal terminated surface, depending upon the direction of the charge transfer [1]. (b) h-BN monolayer on Ni(111) : realization of a potential catalyst for CO oxidation [2]. (c) $MoSe_2$ monolayer on Ni(111) and Cu(111) : modulation of electronic, magnetic and chemical properties [3]

References:

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