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SEMINAR ZAVODA ZA TEORIJSKU FIZIKU

(Zajednički seminari Zavoda za teorijsku fiziku,
Zavoda za eksperimentalnu fiziku IRB-a i Fizičkog odsjeka PMF-a)

Van der Waals interaction on surfaces - three stories

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Abstract:

Ubiquitous van der Waals forces might seem unimportant when compared to much stronger chemical bindings. However in certain situations there are rather unexpected effects caused by vdW interactions.

The first two systems include experimental and theoretical study of Cs and Li atoms adsorption on graphene on Ir(111).

Graphene on Ir(111) surface is an interesting system because graphene has almost pristine electronic structure in it due to its weak bonding character to iridum surface. The bonding is almost exclusively of the van der Waals type.

However adding Cs atoms graphene gets doped and and nature of binding changes - especially in the case when the atoms intercalate. Density Functional Theory calculations with standard semilocal functionals (GGA) - fail to reproduce experimental findings even qualitatively. Only when the newly developed nonlocal correlation functional is used (vdW-DF) which includes van der Waals interactions, are the calculations in agreement with experiment, revealing the mechanism of graphene delamination and relamination which is crucial for intercalation and trapping of atoms under the graphene.

Iridium (111) surface has a very well defined surface state (visible as a sharp peak in ARPES measurement). Addition of lithium atoms destroys the coherence of the surface state resulting in vanishing of the ARPES peak. This behavior is well known in surface science and is actually used as a test for surface states. Surprisingly addition of the graphene on top of lithium results in the restoration of the iridium of surface state. Using the DFT calculations we discovered the mechanism responsible for this, which seems to be quite general.

As the last system I will show as a one slide presentation an explanation of the growth of MoS2 on the surface of the sapphire which can not be resolved by standard DFT calculations due to the size of the common unit cell. However simple vdW interaction calculation reveals much more general picture of this type of systems.

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