Institut Ruđer Bošković
ZAVOD ZA TEORIJSKU FIZIKU
Bijenička c. 54
Zagreb, Hrvatska

SEMINAR ZAVODA ZA TEORIJSKU FIZIKU

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

Graphene on Ir(111), adsorption and intercalation of Cs and Eu atoms

Predrag Lazić
ZTF, IRB

Datum: srijeda, 30. travnja 2014.
Vrijeme : **11:00 sati c.t.**
Mjesto: IRB, dvorana **I** krila

Abstract:

Experimental and theoretical study of Cs and Eu atoms adsorption on graphene on Ir(111) will be presented. 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 or Eu 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, revelaing the mechanism of graphene delamination and relamination which is crucial for intercalation and trapping of atoms under the graphene.

Voditeljica seminara:
Kornelija Passek-Kumerički
$\langle passek@irb.hr \rangle$