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NEBRASKA CENTER FOR MATERIALS AND NANOSCIENCE
2015 SEMINAR SERIES PRESENTS

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Dr. Predrag Lazic

Department of Physics, University of Buffalo

Graphene on Ir(111): Adsorption and intercalation of Cs and Eu atoms

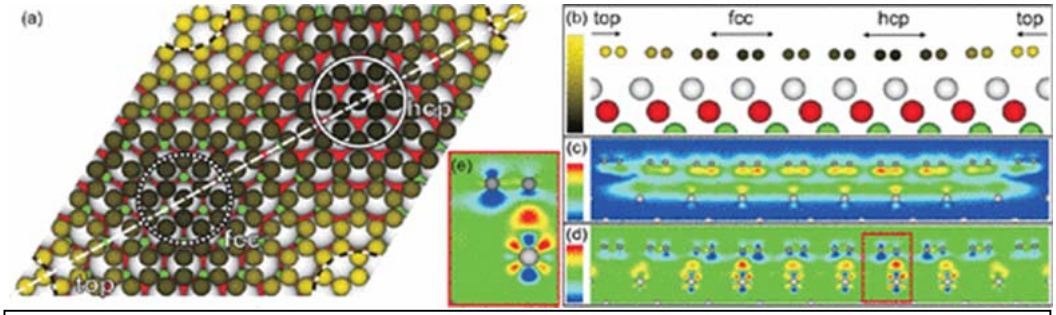

Figure: (a,b) Graphene adsorbed on Ir(111); typical moire pattern is visible (10x10 over 9x9). (c) Nonlocal binding energy contribution. (d) Charge transfer pattern: red (blue) corresponds to electron accumulation (depletion). (e) Enlarged region in red square in panel (d).

Experimental and theoretical study of the adsorption of Cs and Eu atoms on graphene/Ir (111) will be presented [1,2]. In this system graphene has an almost pristine electronic structure due to its weak, almost exclusively van der Waals, bonding to the iridium surface. However, the addition of Cs or Eu atoms leads to charge doping and changes the character of bonding, especially when those atoms intercalate. Density functional theory calculations with standard semilocal functionals (GGA) fail to reproduce the experimental findings even qualitatively. Only when the newly developed nonlocal correlation functional (vdW-DF) including van der Waals interaction is used, are the calculations brought in agreement with experiment. The results reveal the mechanism of graphene delamination and relamination, which is crucial for the intercalation and trapping of atoms under the graphene sheet.

[1] M. Petrovic et al., Nat. Commun. 4, 2772 (2013). [2] S. Schumacher et al., Nano Lett. 13, 5013 (2013).

Dr. Predrag Lazic received his PhD in 2007 from the University of Zagreb (Croatia) in the field of *ab initio* calculations. From 2012 he has held a permanent research scientist position at Rudjer Boskovic Institute in Zagreb. In 2010 he started a software spin-off company Artes Calculi, based on the Robin Hood electrostatic solver. Dr. Lazic has published more than 50 papers in peer-reviewed journals and currently is at the University of Buffalo on a study leave.

Host:
Dr. Kirill Belashchenko
Department of Physics & Astronomy

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Wednesday, April 15, 4:00 pm
136 Jorgensen Hall

3:45 pm - Refreshments served in Jorgensen Atrium