Seminář odd. 26
Tenkých vrstev a nanostruktur

Fyzikální ústav AVČR, Cukrovarnická 10, Praha 6

datum: 30. 5. 2017 úterý

čas: 10:00

místnost: knihovna, budova A, 1.p.

TÉMA

Tailoring graphene electronic, chemical and mechanical properties: interaction with metals, Moire Patterns and the role of defects

Rubén Pérez

Scanning Probe Microscopy Theory & Nanomechanics Group ; Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain , http://www.uam.es/spmth/

The talk will start with a brief summary of the research activity of the SPMTH group, in particular, our recent developments to describe tip-sample transport and interactions for the simulation of STM and AFM [1,2], reducible oxides for catalysys and optoelectronics [3], graphene edge states and vacancy-induced magnetism [4], and the challenges involved in the imaging of surfaces and large biomolecules in their native liquid environment [5,6].

After that, I'll focus in the ability of graphene to corrugate and how the interplay of this structural modulation with the interaction with metal substrates can be exploited to taylor its electronic and chemical properties. We have combined high-resolution STM experiments by different groups and our DFT/STM calculations to challenges some of established ideas for G-metal systems. Experiments in strongly interacting G/Rh(111) conclusively prove the formation of different moiré structures with a wide distribution of surface periodicities. A proper simulation of the current beyond the standard Tersoff-Hamman approach is needed to reproduce quantitatively the trends observed in the STM apparent corrugation. Based on this agreement, we discuss the relative contribution of strain, corrugation and G-metal binding to stabilize the observed moires [7]. We prove the enhanced reactivity of certain Moire areas and show how they contribute to oxygen intercalation, a process that converts a strongly coupled system into a freestanding like p-doped graphene layer [8].

In G/Cu, we have demonstrated that STM can selectively visualize either the graphene layer, the substrate underneath or even both at the same time and exploited this tunable transparency to provide a comprehensive picture of the G-metal coupling with atomic precision and high energy resolution [9], with important implications for the accurate description of van der Waals interactions. Our calculations explain the tunable transparency in terms of the short out-of-plane extension of the graphene electronic states, suggesting that it should apply to a good number of graphene/substrate systems.

Finally, we investigate the influence of defects in the thermal expansion coefficient (TEC) of suspended graphene membranes. Experiments show that low densities of monovacancies reduce the graphene TEC up to one order of magnitude. Our molecular dynamics simulations reproduce the observed trend and show that TEC reduction is due to the suppression of out–of–plane fluctuations caused by the strain fields created by monovacancies in their surrounding areas [10]. These results highlight the key role of defects in the properties of "real-life" graphene and pave the way for future electronic and mechanical defect engineering.

[1] M. Ellner et al, Nano Letters 16, 1974 (2016).
[2] H. Monig et al, ACS Nano 10 1201 (2016).
[3] O. Stetsovych et al, Nature Communications 6, 7265 (2015).
[4] L. Rodrigo et al., Carbon 103, 200 (2016).
[5] J. G. Vilhena et al, ACS Nano 10, 4288 (2016).
[6] J. G. Vilhena et al, Nanoscale 8, 13436 (2016).
[7] A. Martin-Recio et al., Nanoscale 7, 11300 (2015).
[8] C. Romero-Muñiz et al., Carbon 101, 129 (2016); and ACS Nano (submitted).
[9] H. Gonzalez-Herrero et al., ACS Nano 10, 5131 (2016).
[10] G. Lopez-Polin et al., Carbon 116, 670 (2017).

odborný garant: *Ing. Pavel Jelínek, Ph.D.*