The Hebrew University Center
for Nanoscience & Nanotechnology

Nano Seminar

Two-dimensional oxides as new catalytic materials

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Abstract:

Charging of supported clusters on oxide films can occur spontaneously for films of thickness of 1-2 nm via direct tunneling from the metal support [1,2]. This effect, which has been demonstrated for the case of gold atoms and clusters, can significantly modify the shape and chemical reactivity of supported metal clusters [1,2]. The presence of extra charge on the supported metal nanoparticle can have significant effects on catalytic reactons. Thin oxide films can also become active catalysts thanks to their structural flexibility [3] or nanoporosity [4]. Activation of supported metal clusters can be obtained also by doping an oxide film with transition metal atoms incorporated in the inner layers [5-8]. We will discuss the ability of Mo (Cr) impurities in a CaO (MgO) matrix to act as charge donors to adsorbed gold. Whereas CaO_{Mo} features a robust electron donor characteristic, MgO_{Cr} is electrically inactive due to the different stability of various oxidation states. Based on our findings, we develop general rules on how to optimize the electron-donor characteristics of doped oxide materials and thin films and how this can be used to tune the catalytic properties of supported nanoparticles.

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[3] Q. Pan, X. Weng, M. Chen, L. Giordano, G. Pacchioni, C. Noguera, J. Goniakowski, S. Shaikhutdinov, H.-J. Freund, "Enahanced CO oxidation on metal/oxide interface: from ultrahigh vacuum to near-atmospheric pressures", *ChemCatChem*, 7, 2620-2627 (2015).
[4] P. Schlexer, G. Pacchioni, R. Wlodarczyk, J. Sauer, "CO adsorption on a silica bilayer supported on Ru(0001)", *Surface Science*, 648, 2-9 (2016).
[5] X. Shao, S. Prada, L. Giordano, G. Pacchioni, N. Nilius, H.-J. Freund, "Shape control of metal adparticles via doping of the oxide support: An STM and DFT study", *Angew. Chem. Int. Ed.*, 50, 11525 (2011).
[6] F. Stavale, X. Shao, N. Nilius, H.-J. Freund, S. Prada, L. Giordano, G. Pacchioni, "Transition metal dopants and the electron donor characteristic of oxide surfaces", *J. Am. Chem. Soc.*, 134, 11380 (2012).
[7] S. Prada, L. Giordano, G. Pacchioni, "Charging of gold atoms on doped MgO and CaO: identifying the key parameters by DFT calculations", *J. Phys. Chem. C*, 117, 9943 (2013).
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Gathering & Refreshments at 10:50

Please contact Alexandra Bannych at 6584919 if you are interested in meeting the lecturer.

Tuesday, Apr 4th 2017, 11:00 at the Seminar Hall

Los Angeles Building, entrance floor.