NanoLab Talk

Monday, 29th october, 2018 – 16.00

Seminar Room 1° floor

Department of Energy – Cesnef (Building 19) via Ponzio 34/3 Milan

Politecnico di Milano

"Modelling Oxide Surfaces at the 2D Limit"

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Abstract:

In this seminar, the role of first-principles simulations in elucidating structural properties and chemical reactivity of metal-supported oxide thin films will be discussed. Thin oxide films supported on metals represent an interesting class of materials for many applications, spanning from microelectronics to heterogeneous catalysis. From the chemist's perspective, the most relevant aspect of these systems is perhaps the spontaneous charge transfer taking place at the metal/oxide interface, which strongly influences the adsorptive properties and reactivity at the oxide surface. Computer simulations can achieve a reliable description of the structural details and charge state of adsorbed species on oxide thin films, relating the oxide/support interplay to the surface chemical activity. This was first seen in the case of gold single atoms and small clusters adsorbed on a simple model system of metal-supported ionic oxide, namely Ag- or Mo-supported MgO.[1] Interestingly, similar effects have been recently observed also in the case of a real catalyst employed in industrial catalytic synthesis of methanol, namely a ZnO bilayer supported on Cu.[2]
However, there are critical aspects to be considered when simulating complex metal-oxide interfaces. On the one hand, calculations on these systems are often computationally demanding, due to the large dimension of the supercells required to reduce the strain arising from the metal/oxide lattice mismatch. On the other hand, it is not trivial to find a computational method describing equally well the metallic and the oxidic parts of the interface and still being efficient enough to treat large systems.

References

[1] Ricci et al., Phys. Rev. Lett. 2006, 97, 036106−4.

[2] Thang et al., ACS Catal. 2018, 8, 4110.

About the speaker:

Dr. Sergio Tosoni is a research associate at the Materials Science Department, University of Milano - Bicocca. He received his PhD in Chemistry at the University of Torino in 2007. He then held Postdoc positions at the Humboldt University, Berlin, and the University of Barcelona. His main research interests concern first-principles simulations of catalytic and photocatalytic properties of oxide surfaces, metal-oxide interfaces, adsorption and weak interactions.

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