Ph.D. Course in Materials Science and Nanotechnology

University of Milano-Bicocca, Department of Materials Science, via Cozzi 55, 20125 Milano

April 4, 2018 – 4.00 p.m.

Seminar room - Department of Materials Science U5

Francesca Baletto

Physics Department, King's College London

Design of nanocatalysts: hype or hope?

In this talk, I revise the concept of nanoparticles' design for target applications starting from an accurate analysis of their geometrical features [1]. From this point of view, thermal activated rearrangements and phase changes in metallic nanoparticles acuire a new and stronger meaning [2]. After a brief introduction on the numerical tools we have developed, I address the need to include those effects to predicting chemo-physical properties of nanosized metallic or bimetallic objects. As paradigmatic example, I show the prediction of optimal Pt-based nanocatalyts for oxygen reduction reaction [3].

[1] GG Asara, et al. ACS Catalysis 6:4388 (2016); C. DiPaola et al. Nano Letters 16:2885 (2016); C. DiPaola et al. Nanoscale 9:15658 (2017); C. DiPaola et al. PCCP 13:7701 (2011); JBA Davis et al. JPCA 119:9703 (2015)

[2] D. Schebarchov, et al. Nanoscale 10:2004 (2018); K. Rossi and F. Baletto PCCP 19:11057 (2017); K. Rossi et al. JPCM 29:145402 (2017); A. Gould et al. JPCL 7:4414 (2016); L. Pavan et al. JCP 143:184304 (2015)

[3] GG. Asara et al. submitted; D. Schimdt's MSci thesis, King's College London, April 2018.

PhD students and all interested in the seminar are kindly invited to participate.

The PhD Coordinator

Prof. Marco Bernasconi