NIS Colloquium in honor of Alessio Meyer

Simulation vs Experiment: Examples of fruitful interplay in Solid State and Surface Science

Torino 17 December 2010

Dipartimemto Chimica IFM

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Alessio Meyer was a second-year PhD student at the Theoretical Chemistry Group in Torino, when he suddenly and unexpectedly died on 23/12/2009. During his brief but intense scientific activity, he was deeply involved in the clever use of advanced simulation tools and in the development of new ones for application in Solid State Physics and Surface Science, which happened in a constant interaction with experimentalists. This Colloquium in his honor aims precisely at showing how important and fruitful the interplay between experiment and simulation is, through examples provided by scientists who interacted more or less directly with him. The topics selected mainly concern two areas of advanced research where Alessio was specially involved: the characterization of new two-dimensionally ordered phases of oxides supported on metals, and the comprehension of the structural, vibrational, dielectric and magnetic properties of pure and doped garnets.

Friday 17th (morning)

9:00	**Cesare Pisani** (U. Torino)	**Introduction**
9:15	**Gaetano Granozzi** (U. Padova)	**Titania at nanoscale: what is at the bottom**
10:00	**Stefano Agnoli** (U. Padova)	**Nano-oxides of relevance in catalysis: A surface science approach**
10:30	**Paola Finetti** (U. Firenze)	**The role of O and N induced Cu(100) surface restructring in the self-assembling of nanostructured oxides and nitrides**

11:00		**Coffee break**
11:30	**Gianfranco Pacchioni** (U. Milano Bicocca)	**Chemistry on oxide surfaces and thin films: when theory and experiment meet together**
12:10	**Lorenzo Maschio, Valentina Lacivita, Mauro Ferrero, Migen Halo, Anna Ferrari** (U. Torino)	**Testimonies from young scientists and collaborators of Alessio**
13:10		**Lunch (Catering)**

Friday 17th (afternoon)

14:30	**Philippe D'Arco** (UPMC Paris)	**Counting and finding independent configuraions in disordered or substitutional crystalline systems**
15:00	**Michele Catti** (U. Milano Bicocca)	**Simulation of order-disorder in solids with the CRYSTAL code: the case of β-$LiFeO_2$**
15:30	**Carlo Lamberti** (U. Torino)	**Combined XRPD, EXAFS and periodic ab initio approaches to disclose the complex structure of UiO-66 Metal-Organic Framework**
16:00	**Roberto Dovesi** (U. Torino)	**Working with Alessio Meyer on the CRYSTAL code**