UniCat Special Seminar

Unifying Concepts in Catalysis

updates of events on www.unicat.tu-berlin.de

Monday, September 16th, 2013 at 2:00 pm

Lecturer: **Dr. Matteo Maestri**, Assistant professor, Laboratory of Catalyis and Catalytic Processes (LCCP), Energy Department, Politechnico di Milano, Italy

Title: ***A first-principles approach to system complexity in heterogeneous catalysis***

Abstract: The atomic-scale understanding of a catalytic process is crucial for the rational development of new and improved catalytic technologies. It requires the first-principles identification of the catalytic cycle, which is an intrinsic multiscale property of the reacting system. In this talk, I will present recent results from my group on first-principles hierarchical approaches for the multiscale analysis of complex catalytic processes. This methodology turns out to be the most efficient way to integrate the various levels of theory at the different scales into one multiscale simulation, in an effective seamless flow from the atoms to the reactor.

Find more about Dr. Maestri on: http://www.catalyticfoam.polimi.it/ or http://www.energia.polimi.it/english/department/scheda_persona.php?id=180

Lecturer: **Dr. Geoffroy Hautier**, Institute of Condensed Matter and Nanosciences (IMCN), Nanoscopic Physics (NAPS), Université Catholique de Louvain, Belgium

Title: ***Accelerating materials discovery through high-throughput computing and the Materials Project***

Abstract: Many essential materials properties can nowadays be computed through *ab initio* methods. When coupled with the exponential rises in computational resources, this predictive power provides the opportunity for large-scale computational searches for new materials in many technological fields. Tens of thousands of compounds can be screened by their computed properties focusing experiments on the most promising candidates.
In my talk, I will outline some of the challenges and opportunities of this new approach focusing on a few key areas such as Li-ion batteries and transparent conducting oxides. I will also present the Materials Project: a general freely accessible database of high-throughput computed properties.

Find more about Dr. Hautier on: http://www.mendeley.com/profiles/geoffroy-hautier/ or http://www.materialsproject.org

---

Organizer: **Prof. Matthias Driess (TUB)**

Venue: **TU Berlin, Gerhard Ertl Center, Building BEL, Marchstraße 6, 10587 Berlin, Meeting Room BEL 301**

Coffee and tea will be served thirty minutes prior to the lecture start.
Guests are cordially invited to attend!

Prof. Dr. Matthias Driess, Chair of the Cluster of Excellence UniCat