Workshop IV: Physical Frameworks for Sampling Chemical Compound Space

Monday May 16, 2011

8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*

9:00–9:50 **Weitao Yang** (Duke University)
Gradient-based Optimization for Molecular Design

10:00–10:15 *Break*

10:15–11:05 **Dario Alfe** (University College London)
Composition of the Earth's core from ab-initio calculation of chemical potentials

11:15–11:30 *Break*

11:30–12:20
TBA

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **David Beratan** (Duke University)
Coupling Theoretical Explorations in Chemical Space to Synthesis

3:30–4:00 *Break*

4:00–4:50 **Carlos Cardenas** (University of Chile)
Chemical reactivity descriptors applied to the problem of finding optimal doping positions of small metal clusters

5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday May 17, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Igor Abrikosov** (Linköping University)
MAGNETIC EFFECTS IN SIMULATIONS OF STRUCTURAL TRANSFORMATIONS BELOW AND ABOVE THE MAGNETIC TRANSITION TEMPERATURE

10:00–10:15 *Break*

10:15–11:05 **Edward Maginn** (University of Notre Dame)
On the use of gradual transformation methods in computing phase behavior

11:15–11:30 *Break*

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11:30–12:20 **David Kofke** (SUNY Buffalo)
Some Recent Advances in Free Energy and Sampling Methods for Crystals, Mixtures and Coexisting Phases

12:30–2:00 *Lunch (on your own)*

2:00–2:50 **Alejandro Toro-Labbe** (Pontificia Universidad Catolica de Chile)
Toward a Complete Characterization of the Mechanism of Chemical Reactions

3:00–3:15 *Break*

3:15–4:05 **Ping Liu** (Brookhaven National Laboratory)
Theoretical insight into heterogeneous catalysis

4:15–4:30 *Break*

4:30–5:20 **Jeffery Saven** (University of Pennsylvania)
Theoretical approaches for protein sequence ensembles with applications to design

Wednesday May 18, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Herschel Rabitz** (Princeton University)
Why is Chemical Synthesis and Property Optimization Easier than Expected?

10:00–10:15 *Break*

10:15–11:05 **Jochen Blumberger** (University College London)
Towards a computational design of an oxygen tolerant H2 converting enzyme

11:15–11:30 *Break*

11:30–12:20 **Peter Wipf** (University of Pittsburgh)
Synthetic Explorations of Heterocyclic Diversity

12:30–2:00 *Lunch (on your own)*

2:00–2:50 **Clemence Corminboeuf** (École Polytechnique Fédérale de Lausanne (EPFL))
Computational Design of Molecular Properties: Spotlight on Accuracy and Electronic Tuning

3:00–3:15 *Break*

3:15–4:05 **Ivano Tavernelli** (École Polytechnique Fédérale de Lausanne (EPFL))
Ab-initio methods for molecular design

4:15–4:30 *Break*

4:30–5:20 **Alejandro Perez Paz** (New York University)
Path integral computation of quantum free energy differences due to alchemical transformations

Thursday May 19, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Toon Verstraelen** (Ghent University)
Faster potential energy surfaces: the 'art' of making force fields

10:00–10:15 *Break*

10:15–11:05 **Nigel Wilding** (University of Bath)
Structure and phase behavior of highly size-asymmetrical fluid mixtures

11:15–11:30 *Break*

11:30–12:20 **Peter Minary** (Stanford University)
Conformational Optimization and Sampling Along Natural Coordinates

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Marialore Sulpizi** (Johannes Gutenberg-Universität Mainz)
Structure and reactivity of interfaces from Density-Functional Theory simulations

3:30–4:00 *Break*

4:00–4:50 **Markus Reiher** (Swiss Federal Institute of Technology of Zurich)
The Inverse Quantum Chemical Approach to Molecular Vibrational Properties

Friday May 20, 2011

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Paul Ayers** (McMaster University)
Modeling Molecular and Macromolecular Acidity with Quantitative Property-Activity Relations and Machine Learning

10:00–10:15 *Break*

10:15–11:05 **Michael Deem** (Rice University)
A Database of New Zeolite-Like Materials

11:15–11:30 *Break*

11:30–12:20 **Olivier Michielin** (Swiss Institute of Bioinformatics)
Exploring the chemical space of small molecule cancer therapies using a fragment based approach

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Sameer Varma** (Illinois Institute of Technology)
Biological mechanisms for exploiting chemical diversity

3:30–4:00 *Break*

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4:00–4:50 **Michel Cuendet** (New York University)
Dissecting protein-protein interactions and side chain cooperativity.