



INSTITUTE FOR PURE AND APPLIED MATHEMATICS  
Los Angeles, California

# Navigating Chemical Compound Space for Materials and Bio Design

● **March 14 – June 17, 2011**

**ORGANIZING COMMITTEE:** Jean-Loup Faulon (Université d'Évry-Val d'Essonne), William Hart (Sandia National Labs), Kendall Houk (UCLA), Peter Jones (Yale), Steven Lustig (DuPont), Tamar Seideman (Northwestern), Mark Tuckerman (NYU), Anatole von Lilienfeld (Sandia National Labs)

## ● Scientific Overview

Chemical compound space (CCS) is the combinatorial set which encompasses all chemical compounds. It can be viewed as the high dimensional space spanned by all the possible stoichiometries and configurations of electrons and atomic nuclei which form molecular or condensed matter. Due to the combinatorial nature of CCS, systematic screening for interesting properties or even simple enumeration is beyond any computational capacity. But CCS provides a natural framework in which to construct rigorous mathematical tools for the development of direct and inverse quantitative structure-property relationships, which can be applied to challenges in Materials and Bio design. Diverse scientific areas are involved, which benefit from historically grown experimental insights as well as advances made in theoretical and computational sciences. They include statistical mechanics, liquid and solid state physics, quantum chemistry, graph theory, molecular physics, condensed matter physics, optimization algorithms, data mining, statistical analysis, and others.

## ● Workshop Schedule

- Chemical Compound Space Tutorials, March 15-18, 2011
- Workshop 1: Design of Drugs and Chemicals that Influence Biology, April 4-8, 2011
- Workshop 2: Optimization, Search and Graph-Theoretical Algorithms for Chemical Compound Space, April 11-15, 2011
- Workshop 3: Materials Design in Chemical Compound Space, May 2-6, 2011
- Workshop 4: Physical Frameworks for Sampling Chemical Compound Space, May 16-20, 2011
- Culminating Workshop at Lake Arrowhead Conference Center, June 12-17, 2011

## ● Participation

This long program will bring together senior as well as junior researchers of diverse scientific communities, which are involved in addressing the question of how to best navigate CCS, such that they can discuss current bottlenecks with each other and, in particular, with the applied mathematics community. It is expected lead to fruitful collaborations where all participants benefit largely from mathematical insights on their specific optimization and design problems.

Full and partial support for long-term participants is available. We are especially interested in applicants who intend to participate in the entire program, but will consider applications for shorter periods. Funding is available to participants at all academic levels, though recent PhDs, graduate students, and researchers in the early stages of their careers are especially encouraged to apply. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM's mission and we welcome their applications. More information and a link to an application are available online.

● [www.ipam.ucla.edu/programs/ccs2011](http://www.ipam.ucla.edu/programs/ccs2011)



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