KI-Net: Kinetic description of emerging challenges in multiscale problems of natural sciences

An NSF Research Network in Mathematical Sciences

Conference Announcement

Mathematical and Computational Methods in Quantum Chemistry

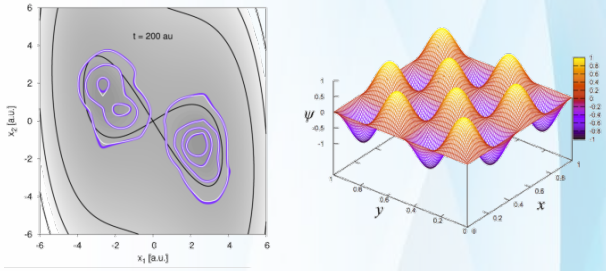
May 13-16, 2016

Department of Chemistry
Yale University

Organizers

Victor Batista	Yale University
Shi Jin	University of Wisconsin - Madison
Qin Li	University of Wisconsin - Madison
Jianfeng Lu	Duke University
Weitao Yang	Duke University

In recent years, the area of mathematical and computational aspects of quantum chemistry has undertaken a rapid development. The interplay between applied mathematics and quantum chemistry is important in generating intriguing new research directions for applied mathematics, in enhancing the understanding of models from quantum chemistry, and in advancing the develeopment of efficient algorithms. This workshop will focus on studying recent developments and open challenges in this area, and on strengthening the interactions between applied mathematician and theoretical chemists.



Goals

This workshop will bring together researchers with diverse expertise on mathematical and numerical methods in quantum chemistry. Our goal is to stimulate interdisciplinary discussions between applied mathematicians and theoretical chemists, with a particular focus on theoretical, mathematical and computational challenges from quantum chemistry. Emphasis will be placed on multiscale problems, quantum-classical coupling, mean-field equations, dimensional reduction, etc.

For more information and to apply: www.ki-net.umd.edu

Confirmed Participants

Wei Cai	University of North Carolina - Charlotte
Eric Cances	Ecole des Ponts and INRIA
Roberto Car	Princeton University
Dangxing Chen	University of North Carolina - Chapel Hill
Qiang Cui	University of Wisconsin - Madison
Di Fang	University of Wisconsin - Madison
Prateek Goel	University of Waterloo
George A. Hagedorn	Virginia Tech
Michael Herman	Tulane University
Kenneth Jung	Yale University
Yosuke Kanai	University of North Carolina - Chapel Hill
Xiantao Li	Penn State University
Lin Lin	University of California, Berkeley
Jian Liu	Peking University
Yvon Maday	University of Paris VI
Nancy Makri	University of Illonois - Urbana Champaign
Dionisios Margetis	University of Maryland
Jose A. Morales Escalante	The University of Texas - Austin
Qian Niu	The University of Texas - Austin
Tomoki Ohsawa	The University of Texas - Dallas
Oleg Prezhdo	University of Southern California
Prashant Rai	Sandia National Laboratories
Sihong Shao	Peking University
Joseph Subotnik	University of Pennsylvania
Eitan Tadmor	University of Maryland
Cesare Tronci	University of Surrey
John Tully	Yale University
Alexander Watson	Columbia University
Qin Wu	Brookhaven National Lab
Dequan Xiao	University of New Haven
Vivek K. Yadav	Temple University
Chao Yang	Lawrence Bekerley National Lab
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KI-Net Hubs

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