



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

An NSF Research Network in Mathematical Sciences



<b>Friday, May 13</b>	
<b>MORNING SESSION</b>	<b>Chair:</b> Victor Batista
8:30 – 9:20	<b>Registration and Breakfast – Sloane Physics Lab</b>
9:20 - 9:30	<i>Welcoming Remarks</i>
9:30 - 10:10	<b>Yvon Maday</b> (University of Paris VI) A Posteriori Quantification of Model/discretization/solution Method Errors for Electronic Structure Calculations
10:15 - 10:55	<b>Michael Herman</b> (Tulane University) An Approximate Semiclassical Method that Uses Real Valued Trajectories for Time Dependent Tunneling Calculations
11:00 - 11:30	<b>COFFEE BREAK</b>
11:30 - 12:10	<b>Aihui Zhou</b> (Chinese Academy of Sciences) A Parallel Orbital-updating Approach for Electronic Structure Calculations
12:15 - 2:00	<b>LUNCH</b> at <b>Charlie's Place</b> located in the <b>Yale School of Management, 165 Whitney Ave.</b> (short walk)
<b>AFTERNOON SESSION</b>	<b>Chair:</b> Shi Jin
2:00 - 2:40	<b>Chao Yang</b> (Lawrence Berkeley National Laboratory) Fast Algorithm for Estimating Absorption Spectrum in Linear Response TDDFT
2:45 – 3:25	<b>Joseph Subotnik</b> (University of Pennsylvania) A Mixed Quantum-Classical View of Surface Hopping
3:30 - 4:00	<b>COFFEE BREAK</b>
4:00 - 4:40	<b>Yosuke Kanai</b> (University of North Carolina, Chapel Hill) Numerical implementation and application of real-time TDDFT in large-scale simulations
4:45 – 5:25	<b>Xiantao Li</b> (Pennsylvania State University) Atom relaxations in the electron-structure calculation

<b>Saturday, May 14</b>	
<b>MORNING SESSION</b>	<b>Chair:</b> Jianfeng Lu
8:30 – 9:20	<b>Breakfast</b>
9:30 - 10:10	<b>Shi Jin</b> (University of Wisconsin at Madison) Semiclassical computational methods for quantum dynamics with band-crossing
10:15 - 10:55	<b>Oleg Prezhdo</b> (University of Southern California) Nonadiabatic Molecular Dynamics with Time-Domain Density Functional Theory
11:00 - 11:30	<b>COFFEE BREAK</b>
11:30 - 12:10	<b>Victor Batista</b> (Yale University) Time Sliced Thawed Gaussian Propagation for Quantum Dynamics Simulations
12:15 - 2:00	<b>LUNCH</b> on the <b>third floor lounge of Sloane Physics Lab</b>
<b>AFTERNOON SESSION</b>	<b>Chair:</b> Weitao Yang
2:00 - 2:40	<b>Lin Lin</b> (University of California Berkeley) Adaptively compressed exchange operator
2:45 – 3:25	<b>Jianfeng Lu</b> (Duke University) Towards a mathematical understanding of surface hopping algorithms
3:30 – 4:00	<b>COFFEE BREAK</b>
4:00 – 5:25	Free time for discussion
6:00 – 9:00	<b>Banquet</b> at <b>Quinnipiac Club</b> , 221 Church Street, New Haven, CT  Banquet Talk by <b>John Tully</b> (Yale University) Adventures with Surface Hopping

<b>Sunday, May 15</b>	
<b>MORNING SESSION</b>	<b>Chair:</b> Jianfeng Lu
8:30 – 9:30	<b>Breakfast</b>
9:30 - 10:10	<b>Weitao Yang</b> (Duke University) Electron Correlation and Excitations from Pairing Matrix Fluctuation and Particle-Particle Random Phase Approximation
10:15 - 10:55	<b>Eric Cancès</b> (Ecole des Ponts and INRIA) A mathematical formulation of the GW method
11:00 - 11:30	<b>COFFEE BREAK</b>
11:30 - 12:10	<b>Nancy Makri</b> (University of Illinois Urbana Champaign) Classical vs. Quantum Decoherence and the Quantum-Classical Path Integral
12:15 - 2:00	<b>LUNCH</b> on the <b>third floor lounge of Sloane Physics Lab</b>
<b>AFTERNOON SESSION</b>	<b>Chair:</b> Shi Jin
2:00 - 2:40	<b>Qian Niu</b> (University of Texas at Austin) Semiclassical electron dynamics in crystals
2:45 – 3:25	<b>Jian Liu</b> (Peking University) A novel quantum dynamics method for thermal correlation functions
3:30 - 4:00	<b>COFFEE BREAK</b>
4:00 - 4:40	<b>Alexey Akimov</b> (SUNY Buffalo) TBA
4:45 – 5:25	<b>Zhennan Zhou</b> (Duke University) Bloch dynamics with second order Berry phase correction

<b>Monday, May 16</b>	
<b>MORNING SESSION</b>	<b>Chair:</b> Victor Batista
8:30 – 9:00	<b>Breakfast</b>
9:00 - 9:40	<b>Qiang Cui</b> (University of Wisconsin at Madison) Hybrid QM/MM methods for biophysics and solid/liquid interfaces
9:45 - 10:30	<b>George Hagedorn</b> (Virginia Tech) A Numerical Algorithm for Semiclassical Dynamics in Several Space Dimensions
10:30 - 11:00	<b>COFFEE BREAK</b>
11:00 - 11:40	<b>Dionisios Margetis</b> (University of Maryland College Park) Aspects of many-Boson dynamics
11:45 - 12:30	<b>Sihong Shao</b> (Peking University) A Computable Branching Random Walk for the Wigner Quantum Dynamics
	<b>CLOSING</b>

