Jerusalem Nonadiabatica 2018 Program

MONDAY 12 MARCH 2018

I		Chair: **Robert Englman**, Ariel University	
8:50	9:00	Welcome, opening remarks	Roi Baer
9:00	9:30	The H3++ Molecular System as a Cornerstone for Building Molecules During the Big Bang	**Michael Baer**, Soreq Nuclear Center and Fritz Haber Center, The Hebrew University of Jerusalem, Israel
9:30	10:00	Quantum Nonadiabatic Dynamics in the Moving Crude Adiabatc Representation	**Artur Izmaylov**, University of Toronto, Canada
10:00	10:30	Jahn-Teller effect among electronic resonant states of H3	**Asa Larson**, University of Stockholm, Sweden
10:30	11:00	Coffee	
11:00	11:30	Exact factorization for nonadiabatic dynamics	**Eberhard K. U. Gross**, Max Planck Institute for Microstructure Physics, Halle, Germany, and Fritz Haber Center, The Hebrew University of Jerusalem, Israel
11:30	12:00	Nonadiabatic Energy Transfer	**Troy van Voorhis**, Massachusettes Institute of Technology, Massachusettes, USA
12:00	12:30	Rigorous Trajectory-Based Methods for Simulating Nonadiabatic Dynamics	**Craig Martens**, University of California Irvine, USA
12:30	15:00	Lunch	
II		Chair: **Dorit Shemesh**, Fritz Haber Center, The Hebrew University of Jerusalem, Israel	
15:00	15:30	New electronic structure tools for modeling non-adiabatic processes	**Anna Krylov**, University of Southern California, USA
15:30	16:00	Excited state dynamics in Proteorhodopsin	**Igor Schapiro**, Fritz Haber Center, The Hebrew University of Jerusalem, Israel
16:00	16:30	CASPT2 non-adiabatic dynamics	**Toru Shiozaki**, Northwestern University, Illinois, USA
16:30	17:00	Coffee	
17:00	17:30	Time evolution of the Landau-Zener problem under weak measurement	**Abraham Nitzan**, University of Pennsylvania, USA and Tel Aviv University, Israel
17:30	18:00	Non-Equilibrium Thermodynamics in Open Quantum Systems via The Driven Liouville von Neumann (DLvN) Approach	**Oded Hod**, Tel Aviv University, Israel
18:00		Reception and Poster Session	

TUESDAY 13 MARCH 2018

III		Chair: **Daniel Strasser**, Hebrew University of Jerusalem, Israel	
9:00	9:30	Describing Potential Energy Surfaces around Conical Intersections via Symmetry Breaking and Restoration Techniques	**Gustavo Scuseria**, Rice University, Texas, USA
9:30	10:00	Derivative Couplings, Line Integrals, Fit Coupled Potential Energy Surfaces and the Molecular Aharanov Bohm Effect Revisited	**David Yarkony**, Johns Hopkins University, Maryland, USA
10:00	10:30	Towards quantum simulations for electronic dynamics for small molecules with Multi-Configuration Time-Dependent Hartree (MCTDH)	**Fabien Gatti**, University Paris Sud, France
10:30	11:00	Non-adiabatic coupling in the ozone molecule	**Alexander Alijah**, University of Reims, France
11:00	11:30	Coffee	
IV		Chair**: Igor Rahinov**, The Open University, Israel	
11:30	12:00	Nested Funnels and Nonadiabatic Dynamics in Photosynthesis	**David Jonas**, University of Colorado Boulder, USA
12:00	12:30	Understanding and engineering the vibrational coherence of vision	**Massimo Olivucci**, Universita di Siena, Italy
12:30	13:00	Geometric Phase Effects in Nonadiabatic Tunneling	**Hua Guo**, University of New Mexico, USA
13:00	13:30	Combined Electronic Structure and Quantum Dynamical Analysis for Charge Separation and Singlet Fission	**Hiroyuki Tamura**, The University of Tokyo, Japan
13:30	19:00	Lunchboxes + Tour to old city	
19:00		Festive Dinner	
		On the Occasion of Michael Baer's 80'th Birthday: **Tribute to a Pioneer in Chemical Physics**	Donald J. Kouri, University of Houston, Texas, USA

WEDNESDAY 14 MARCH 2018

V		Chair: **Igor Schapiro**, Fritz Haber Center, The Hebrew University of Jerusalem	
9:00	9:30	Classical Molecular Dynamics Simulations of Electronically Non-Adiabatic Processes	**William Miller**, University of California, Berkeley, California, USA
9:30	10:00	Excited state dynamics with trajectories	**Federica Agostini**, University Paris-Sud, France
10:00	10:30	Full Quantum Direct Dynamics Simulations of Non-adiabatic Photochemistry	**Graham Worth**, University College London, UK
10:30	11:00	Coffee	
11:00	11:30	Isotope effect in a nonadiabatic transition and longer time vibronic coherence	**Raphael D. Levine**, Fritz Haber Center, The Hebrew University of Jerusalem, Israel
11:30	12:00	Light-induced conical intersections	**Ágnes Vibók**, University of Debrecen, Hungary
12:00	12:30	Coupled supersymmetries and associated Fourier-like transforms for a wide class of superpotentials	**Donald J. Kouri**, University of Houston, Texas, USA
12:30	14:30	Lunch	
VI		Chair: **Ester Livshits**, Fritz Haber Center, The Hebrew University of Jerusalem	
14:30	15:00	Time-Dependent Nonadiabatic Markovian Quantum Master Equation	**Ronnie Kosloff**, Fritz Haber Center, The Hebrew University of Jerusalem, Israel
15:00	15:30	Non Adiabatic Phenomena in Open Systems	**Nimrod Moiseyev**, Technion - Israel Institute of Technology, Israel
15:30	16:00	Nonadiabatic Dynamics via The Generalized Quantum Master Equation	**Eitan Geva**, University of Michigan at Ann Arbor, Israel
16:00	16:30	Coffee	
16:30	17:00	Building the World's Greatest Microscope: Revealing the atomic scale dynamics of surface chemistry	**Alec Wodtke**, Max Planck Institute Göttingen, Germany
17:00	17:30	Cooling and Mechanical Stabilization of Molecular Resonant Tunneling Devices	**Uri Peskin**, Technion - Israel Institute of Technology, Israel
17:30	18:00	Mean Field vs Stochastic Approaches to Nonadiabatic Dynamics	**Joe Subotnik**, University of Pennsylvania, USA

THURSDAY 15 MARCH 2018

VII		Chair: **Narayanasami Sathyamurthy**, Indian Institute of Science Education and Research, Mohali, India	
9:00	9:30	Electronic Excited States from Pairing Matrix Fluctuations and Particle-Particle Random Phase Approximation	**Weitao Yang**, Duke University, North Carolina, USA
9:30	10:00	Stochastic GW for thousands of electrons and more	**Daniel Neuhauser**, University of California at Los Angeles, California, USA
10:00	10:30	Beyond Born-Oppenheimer Theories on Molecular Processes and Phase Transitions in Solid States	**Satrajit Adhikari**, Indian Association for the Cultivation of Science, Calcutta, India
10:30	11:00	Coffee	
11:00	11:30	Ultrafast nonadiabatic dynamics in photovoltaic polymer materials: Coherence, delocalization, and disorder	**Irene Burghardt**, Goethe University, Frankfurt, Germany
11:30	12:00	Non-Adiabatic Interaction and the Geometric Phase	**Narayanasami Sathyamurthy**, Indian Institute of Science Education and Research, Mohali, India
12:00	12:30	Nonadiabatic Dynamics Simulations of Organic Materials with Optical Activity	**Mario Barbatti**, Aix-Marseille Université, France
12:30	14:30	Lunch	
VIII		Chair: **Francoise Remacle**, Department of Chemistry, University of Liège, Liège Belgium	
14:30	15:00	Recent advances in nonadiabatic dynamics and applications to nanoscale materials	**Oleg Prezhdo**, University of Southern California, California, USA
15:00	15:30	Probing chromophores for singlet fission by surface hopping simulations.	**Maurizio Persico**, Università di Pisa, Italy
15:30	16:00	Quantum Transitions with Classical Trajectories: A Simple and Rigorous Derivation	**David Tannor**, Weizmann Institute of Science, Israel
16:00	16:30	Coffee	
16:30	17:00	Electron and Nuclear Dynamics Driven by a Coherent Superposition of Electronic Wavefunctions (Implications for Attosecond Spectroscopy)	**Michael Robb**, Imperial College London, UK
17:00	17:30	Time-Domain Quantum Chemistry	**Kazuo Takatsuka**, The University of Tokyo, Japan
17:30	18:00	Tunneling flight time in nonadiabatic transitions.	**Eli Pollak**, Weizmann Institute of Science, Israel