



# Jerusalem Nonadiabatica 2018 Program

**MONDAY 12 MARCH 2018**

I Chair: <b>Robert Englman</b> , Ariel University			
8:50	9:00	Welcome, opening remarks	Roi Baer
9:00	9:30	The H <sub>3</sub> <sup>++</sup> Molecular System as a Cornerstone for Building Molecules During the Big Bang	<b>Michael Baer</b> , Soreq Nuclear Center and Fritz Haber Center, The Hebrew University of Jerusalem, Israel
9:30	10:00	Quantum Nonadiabatic Dynamics in the Moving Crude Adiabatic Representation	<b>Artur Izmaylov</b> , University of Toronto, Canada
10:00	10:30	Jahn-Teller effect among electronic resonant states of H <sub>3</sub>	<b>Asa Larson</b> , University of Stockholm, Sweden
10:30	11:00	Coffee	
11:00	11:30	Exact factorization for nonadiabatic dynamics	<b>Eberhard K. U. Gross</b> , Max Planck Institute for Microstructure Physics, Halle, Germany, and Fritz Haber Center, The Hebrew University of Jerusalem, Israel
11:30	12:00	Geometric Phase Effects in Nonadiabatic Tunneling	<b>Hua Guo</b> , University of New Mexico, USA
12:00	12:30	Rigorous Trajectory-Based Methods for Simulating Nonadiabatic Dynamics	<b>Craig Martens</b> , University of California Irvine, USA
12:30	15:00	Lunch	
II Chair: <b>Dorit Shemesh</b> , Fritz Haber Center, The Hebrew University of Jerusalem, Israel			
15:00	15:30	New electronic structure tools for modeling non-adiabatic processes	<b>Anna Krylov</b> , University of Southern California, USA
15:30	16:00	Excited state dynamics in Proteorhodopsin	<b>Igor Schapiro</b> , Fritz Haber Center, The Hebrew University of Jerusalem, Israel
16:00	16:30	CASPT2 non-adiabatic dynamics	<b>Toru Shiozaki</b> , Northwestern University, Illinois, USA
16:30	17:00	Coffee	
17:00	17:30	Time evolution of the Landau-Zener problem under weak measurement	<b>Abraham Nitzan</b> , 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	<b>Oded Hod</b> , Tel Aviv University, Israel
18:00		Reception and Poster Session	



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### TUESDAY 13 MARCH 2018

III Chair: <b>Daniel Strasser</b> , Hebrew University of Jerusalem, Israel			
9:00	9:30	Describing Potential Energy Surfaces around Conical Intersections via Symmetry Breaking and Restoration Techniques	<b>Gustavo Scuseria</b> , Rice University, Texas, USA
9:30	10:00	Derivative Couplings, Line Integrals, Fit Coupled Potential Energy Surfaces and the Molecular Aharonov Bohm Effect Revisited	<b>David Yarkony</b> , 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)	<b>Fabien Gatti</b> , University Paris Sud, France
10:30	11:00	Non-adiabatic coupling in the ozone molecule	<b>Alexander Alijah</b> , University of Reims, France
11:00	11:30	Coffee	
IV Chair: <b>Igor Rahinov</b> , The Open University, Israel			
11:30	12:00	Nested Funnels and Nonadiabatic Dynamics in Photosynthesis	<b>David Jonas</b> , University of Colorado Boulder, USA
12:00	12:30	Understanding and engineering the vibrational coherence of vision	<b>Massimo Olivucci</b> , Universita di Siena, Italy
12:30	13:00	Nonadiabatic Energy Transfer	<b>Troy van Voorhis</b> , Massachusetts Institute of Technology, Massachusetts, USA
13:00	13:30	Combined Electronic Structure and Quantum Dynamical Analysis for Charge Separation and Singlet Fission	<b>Hiroyuki Tamura</b> , 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: <b>Tribute to a Pioneer in Chemical Physics</b>	Donald J. Kouri, University of Houston, Texas, USA



## Jerusalem Nonadiabatica 2018 Program

### WEDNESDAY 14 MARCH 2018

V Chair: <b>Igor Schapiro</b> , Fritz Haber Center, The Hebrew University of Jerusalem			
9:00	9:30	Classical Molecular Dynamics Simulations of Electronically Non-Adiabatic Processes	<b>William Miller</b> , University of California, Berkeley, California, USA
9:30	10:00	Excited state dynamics with trajectories	<b>Federica Agostini</b> , University Paris-Sud, France
10:00	10:30	Full Quantum Direct Dynamics Simulations of Non-adiabatic Photochemistry	<b>Graham Worth</b> , University College London, UK
10:30	11:00	Coffee	
11:00	11:30	Isotope effect in a nonadiabatic transition and longer time vibronic coherence	<b>Raphael D. Levine</b> , Fritz Haber Center, The Hebrew University of Jerusalem, Israel
11:30	12:00	Light-induced conical intersections	<b>Ágnes Vibók</b> , University of Debrecen, Hungary
12:00	12:30	A New Look at Normal and Anomalous Diffusion	<b>Donald J. Kouri</b> , University of Houston, Texas, USA
12:30	14:30	Lunch	
VI Chair: <b>Ester Livshits</b> , Fritz Haber Center, The Hebrew University of Jerusalem			
14:30	15:00	Time-Dependent Nonadiabatic Markovian Quantum Master Equation	<b>Ronnie Kosloff</b> , Fritz Haber Center, The Hebrew University of Jerusalem, Israel
15:00	15:30	Non Adiabatic Phenomena in Open Systems	<b>Nimrod Moiseyev</b> , Technion - Israel Institute of Technology, Israel
15:30	16:00	Nonadiabatic Dynamics via The Generalized Quantum Master Equation	<b>Eitan Geva</b> , 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	<b>Alec Wodtke</b> , Max Planck Institute Göttingen, Germany
17:00	17:30	Cooling and Mechanical Stabilization of Molecular Resonant Tunneling Devices	<b>Uri Peskin</b> , Technion - Israel Institute of Technology, Israel
17:30	18:00	Mean Field vs Stochastic Approaches to Nonadiabatic Dynamics	<b>Joe Subotnik</b> , University of Pennsylvania, USA



## Jerusalem Nonadiabatica 2018 Program

**THURSDAY 15 MARCH 2018**

VII		Chair: <b>Narayanasami Sathyamurthy</b> , 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	<b>Weitao Yang</b> , Duke University, North Carolina, USA
9:30	10:00	Stochastic GW for thousands of electrons and more	<b>Daniel Neuhauser</b> , 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	<b>Satrajit Adhikari</b> , 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	<b>Irene Burghardt</b> , Goethe University, Frankfurt, Germany
11:30	12:00	Non-Adiabatic Interaction and the Geometric Phase	<b>Narayanasami Sathyamurthy</b> , Indian Institute of Science Education and Research, Mohali, India
12:00	12:30	Nonadiabatic Dynamics Simulations of Organic Materials with Optical Activity	<b>Mario Barbatti</b> , Aix-Marseille Université, France
12:30	14:30	Lunch	
VIII		Chair: <b>Francoise Remacle</b> , Department of Chemistry, University of Liège, Liège Belgium	
14:30	15:00	Recent advances in nonadiabatic dynamics and applications to nanoscale materials	<b>Oleg Prezhdo</b> , University of Southern California, California, USA
15:00	15:30	Probing chromophores for singlet fission by surface hopping simulations.	<b>Maurizio Persico</b> , Università di Pisa, Italy
15:30	16:00	Quantum Transitions with Classical Trajectories: A Simple and Rigorous Derivation	<b>David Tannor</b> , 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)	<b>Michael Robb</b> , Imperial College London, UK
17:00	17:30	Time-Domain Quantum Chemistry	<b>Kazuo Takatsuka</b> , The University of Tokyo, Japan
17:30	18:00	Tunneling flight time in nonadiabatic transitions.	<b>Eli Pollak</b> , Weizmann Institute of Science, Israel