

QAMTS 2017 Program (May 16, 2017)

Saturday May 20

18:00-20:00 Registration and Welcome Reception

Sunday May 21

8:00-8:45 Breakfast

9:00 Welcome, *Bob McMahon*

9:15 Hydrogen Bond Network Rearrangement Dynamics in Water Clusters: Implications for the Liquid, *Richard Saykally, Berkeley*

10:00 The Use of the Bell-Limbach Tunneling Model for the Calculation of Arrhenius Curves of Hydrogen Transfer in Liquids and Solids, *Hans Limbach, Berlin*

10:45-11:15 Coffee

11:15 Hydride Transfer Probed using Mass-Modulated Enzymes and Coenzyme Biomimetics, *Nigel Scrutton, Manchester*

12:00 Influence of Conformation and Environment on Tunnelling Reactions, *Tim Schleif, Joel Mieres Perez, Paolo Costa, and Wolfram Sander, Bochum*

12:45-14:00 Lunch

14:00 Quantum Correlations in Molecular Rotor Systems, *Thomas Halverson and Pierre-Nicholas Roy, Waterloo*

14:45 Including Tunneling in Semiclassical Simulations, *Rubén Meana-Pañeda, Jingjing Zheng, Xuefei Xu, and Donald G. Truhlar, Bethesda*

15:15-15:45 Coffee

15:45 Lipoxygenase as a Model for Vibronically Non-Adiabatic Proton-Coupled Electron Tunneling Near Room Temperature, *Judith Klinman, Berkeley*

16:30 General Algorithm Implementation for Thermal Rates: the Galitherra Software, *David Ferro-Costas and Antonio Fernández-Ramos, Santiago de Compostela*

18:00 Dinner

Monday May 22

8:00-8:45 Breakfast

9:00 Symmetrical Quasi-Classical Model for Classical Molecular Dynamics Simulations of Electronically Non-Adiabatic Processes, *William Miller, Berkeley*

9:45 Translation-rotation Dynamics of Clathrate-confined Dihydrogen Clusters, *Peter Felker, Los Angeles*

10:30-11:00 Coffee

11:00 Manipulating and Probing the Polarisation of a Methyl Tunnelling System by Field-cycling NMR, *Anthony J Horsewill, Bo Zhang, Sabah M.M. Abu-Khumra, and Abdellah Aibout, Nottingham*

11:30 Empirical Valence Bond Studies of Decomposition of Neurotransmitters Catalyzed by Monoamine Oxidases, *Jernej Stare and Janez Mavri, Ljubljana*

12:00 -13:00 Lunch

13:15 Excursion – shuttle bus leaves promptly at 13:15

15:00-17:00 Tour of Frank Lloyd Wright's *Taliesin*, Spring Green, WI

<http://www.taliesinpreservation.org/>

18:15 Approximate time of return to conference hotel

18:30 Dinner

Tuesday May 23

8:00-8:45 Breakfast

9:00 Proton Tunneling in Proteins, *Paul M. Champion, Boston*

9:45 Heavy-atom Tunneling Calculations in Thirteen Organic Reactions: Bell's Formula Matches Multidimensional Tunneling at ≥ 250 K, *Edyta M. Greer, Randy Armas, Dana Walker, Christopher V. Cosgriff, and Charles Doubleday, New York*

10:30-11:00 Coffee

11:00 Tunnelling and Parity Violation in Chiral Molecules: From Theory towards Spectroscopic Experiment and the Evolution of Biomolecular Homochirality, *Martin Quack, Zürich*

11:45 On the use of Quantum Dynamics to Unveil the Complex Photochemistry of Green Fluorescent Protein, *Miquel Moreno, Marc Nadal-Ferret, Ricard Gelabert, and José M. Lluch, Barcelona*

12:30-14:00 Lunch

14:00 Neutron Spectroscopy of Water under Ultra-confinement, *Alexander I. Kolesnikov, Knoxville*

14:45 Molecular Dynamics of Large Systems with Quantum Corrections for Selected Nuclei, *Sophya Garashchuk, Columbia, SC*

15:30 Rovibrational Quantum Dynamics of the Methane-water Dimer, *János Sarka, Attila G. Császár, and Edit Mátyus, Budapest*

16:00-16:30 Coffee

16:30 Isotopically Different Tunneling-Ready-State Structures in Hydride Transfer Reactions in Solution, *Yun Lu, Edwardsville*

17:15 H-Tunneling-Ready-State Structures Obtained from Adjusting Hessian Matrices of Donor-Acceptor Complexes, *Nader Sakhaee and Yun Lu, Edwardsville*

18:30 Conference Banquet
Pyle Center, University of Wisconsin-Madison
Approximately 15-minute walk from conference hotel

Wednesday May 24

8:00-8:45 Breakfast

9:00 The Mechanism of Double-Proton Transfer at Very Low Temperatures, *Antonio Fernández-Ramos, Santiago de Compostela*

9:45 Quantum Transition State Theory, *Timothy J. H. Hele, Ithaca*

10:30-11:00 Coffee

11:00 **The last word:** How Important is Quantum Tunneling in Enzyme Reactions? *Dan T. Major, Ramat-Gan*

11:45 Concluding Remarks, Bob McMahon and Juergen Eckert

12:00 Lunch and departure