XVIth Quantum Reactive Scattering Workshop
4-9. September 2022
Balatonföldvár, Hungary

Program

Monday 05. September 2022.

8:45 Opening

9:00-11:00 Session A Chair: Jonathan N. L. Connor

9:00 Muwen Yang, Sajal Giri and George C. Schatz
Northwestern University, Evanston IL 60208-3113 USA
GETTING CO_2 TO REACT ISN'T EASY: HITTING IT HARD WITH ATOMIC OXYGEN OR WITH HOT ELECTRONS

9:40 Tomás González-Lezana
Instituto de Física Fundamental IFF-CSIC, Serrano 123, 28006 Madrid, Spain
REACTIVE SCATTERING OF ATOM-DIATOM PROCESSES OF ASTROPHYSICAL INTEREST

10:20 Sergio Rampino
Dipartimento di Scienze Chimiche, Università degli Studi di Padova, Padova, Italy
POTENTIAL ENERGY SURFACES FOR QUANTUM REACTIVE SCATTERING: FROM CONSTRUCTION TO ANALYSIS AND USE IN DYNAMICS CALCULATIONS

11:00 Session break

11:20-12:40 Session B Chair: Srihari Keshavamurthy

11:20 J. N. L. Connor[1] and Chengkui Xiahou[2]
[1] Department of Chemistry, University of Manchester, Manchester M13 9PL, UK.
[2] School of Pharmacy, Qilu Medical University, Zibo City 255300, Shandong, PRC.
HOW TO UNDERSTAND STRUCTURE IN THE ANGULAR SCATTERING OF THE STATE-TO-STATE H + HD → H_2 + D REACTION

12:00 E. Akhmatskaya,[1,2] and D. Sokolovski[2,3]
[1] Basque Center for Applied Mathematics (BCAM), Alameda de Mazarredo 14, 48009 Bilbao, Bizkaia, Spain, [2]IKERBASQUE, Basque Foundation for Science, Plaza Euskadi 5, 48009, Bilbao, Bizkaia, Spain, [3]Department of Physical Chemistry, University of the Basque Country, Leioa, 48940, Spain
PADÉ_II, ICS_REGGE, AND DCS_REGGE: COMPUTER PROGRAMS WHICH MAY HELP TO LEARN MORE ABOUT WHAT HAPPENS IN A CHEMICAL REACTION

12:40 Lunch break

14:30-16:10 Session C Chair: Tomás González-Lezana

14:30 Andrea Lombardi
Dipartimento di Chimica, Biologia e Biotecnologie, Unibersità di Perugia, Perugia, Italy
MOLECULAR NETWORKS BY INVARIANT SHAPE COORDINATES AND DEFORMATION INDEXES

Monday 05. September 2022.

15:10 Tibor Győri, Domonkos A. Tasi, Viktor Tajti, Dóra Papp and Gábor Czakó
MTA-SZTE Lendület Computational Reaction Dynamics Research Group, Interdisciplinary Excellence Centre and Department of Physical Chemistry and Materials Science, University of Szeged, Szeged, Hungary
TOOLS FOR AUTOMATED PES DEVELOPMENT: ROBOSURFER AND MANYHF

15:30 Alberto García-Vela
Instituto de Física Fundamental, CSIC, Madrid, Spain
INFLUENCE OF CONICAL INTERSECTIONS IN THE PHOTODISSOCIATION MECHANISMS OF ALKYL RADICALS

16:10 Session break

16:40-18:20 Session D Chair: Stephen J. Klippenstein

16:40 Timo T. Pekkanen,[1] Raimo S. Timonen,[1] György Lendvay,[2] Struan Robertson,[3] and Arkke J. Eskola,[1]
[1] Department of Chemistry, University of Helsinki, P.O. Box 55 (A.I Virtasen aukio 1), Helsinki, 00014, Finland, [2] Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Magyar Tudósok krt 2., Budapest, H-1117, Hungary
[3] Dassault Systèmes, 334 Science Park, Cambridge CB4 0WN, U.K.
OPTIMISING MASTER EQUATION PARAMETERS WITH TRACE FITTING

17:20 Irén Simkó,[1,2] Tamás Szidarovszky,[1] and Attila G. Császár[1,2]
[1] Institute of Chemistry, ELTE Eötvös Loránd University, H-1117 Budapest, Pázmány Péter sétány. 1/A, Hungary, [2] MTA-ELTE Complex Chemical Systems research Group, H-1532 Budapest, P.O. Box 32, Hungary
ROTATIONAL-VIBRATIONAL RESONANCE STATES

18:00 Break

18:30 Dinner

Tuesday 06. September 2022.

9:00-11:00 Session E Chair: Carlo Petrongolo

9:00 A. J. C. Varandas
Department of Physics, Qufu Normal University, China
Department of Physics, Universidade Federal do Espírito Santo, 29075-910 Vitória, Brazil
Coimbra Chemistry Centre, University of Coimbra, 3004-535 Coimbra, Portugal
FROM MOLECULAR SHAPES TO REACTION DYNAMICS

9:40 Prabhash Mahata, Akshaya Kumar Rauta, Subhendu Ghosh and Biswajit Maiti
Department of Chemistry, Inst. of Science, Banaras Hindu University, Varanasi 221005, India
PHOTODISSOCIATION AND NONADIABATIC DYNAMICS OF SMALL ORGANIC MOLECULES

10:20 Tatsuhiro Murakami[1,2] and Toshiyuki Takayanagi[1]
[1]Saitama University, Saitama, Japan, [2]Sophia University, Tokyo, Japan
TWO-STATE REACTIVITY IN Fe-CATALYZED β-HYDROGEN ELIMINATION OF ETHYL CATION

11:00 Session break

Tuesday 06. September 2022.

11:20-12:40 Session F Chair: Gunnar Nyman

11:20 Stephen J. Klippenstein
Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL, USA
RRKM THEORY FOR REACTIVE INTERMEDIATES

12:00 Mihael Eraković[1] and Marko T. Cvitaš[2]
[1]Institute Ruđer Bošković, Zagreb, Croatia, [2]Faculty of Science, University of Zagreb, Zagreb, Croatia
USES OF INSTANTONS IN THE CALCULATIONS OF VIBRATIONAL TUNNELING SPECTRA

12:40 Lunch break

14:30-16:10 Session G Chair: Attila G. Császár

14:30 Gerrit C. Groenenboom, Marijn P. Man, and Tijs Karman
Theoretical Chemistry, Institute of Molecules and Materials, Radboud University, Nijmegen, The Netherlands
ULTRACOLD CHEMISTRY AND COLLISION COMPLEXES

15:10 Grégoire Guillon,[1] Erwan Privat,[1] Pascal Honvault[1], Maxence Lepers[1]
Lab. ICB, Université de Bourgogne/CNRS, Dijon, Burgundy, France
QUANTUM DYNAMICS OF ISOTOPE EXCHANGE REACTIONS : THE OZONE EXAMPLE

15:40 Péter Szabó[1,2] and Magnus Gustafsson[2]
[1]KU Leuven, Leuven, Belgium, [2]Luleå University of Technology, Luleå, Sweden
POLYATOMIC RADIATIVE ASSOCIATION BY QUASICLASSICAL TRAJECTORY CALCULATIONS

16:20 Session break

16:40-18:20 Session H Chair: Antonio J. C. Varandas

16:40 Priyanka Pandey and Srihari Keshavamurthy
[1]Department of Chemistry, Indian Institute of Technology Kanpur, Uttar Pradesh, 208 016, India
DYNAMICAL IMPLICATIONS OF HILLTOPS AND CALDERAS

17:20 János Sarka and Bill Poirier
Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, USA
HITTING THE TRIFECTA: HOW TO SIMULTANEOUSLY PUSH THE LIMITS OF SCHRÖDINGER SOLUTION WITH RESPECT TO SYSTEM SIZE, CONVERGENCE ACCURACY, AND NUMBER OF COMPUTED STATES

18:00 Cangtao Yin, Viktor Tajti, and Gábor Czakó
MTA-SZTE Lendület Computational Reaction Dynamics Research Group, Interdisciplinary Excellence Centre and Department of Physical Chemistry and Materials Science, Institute of Chemistry, University of Szeged, Rerrich Béla tér 1, Szeged H-6720, Hungary
POTENTIAL ENERGY SURFACE DEVELOPMENTS AND DYNAMICS FOR THE REACTIONS OF C_2H_5 WITH HBr AND HI

18:20 Break

18:30 Dinner

Wednesday 07. September 2022.

9:00-11:00 Session I Chair: Uwe Manthe

9:00 Bikram Mandal, Carolin Joy, Dulat Bostan and Dmitri Babikov
Marquette University, Milwaukee, Wisconsin, USA
MQCT – A PROGRAM FOR CALCULATIONS OF INELASTIC SCATTERING OF TWO MOLECULES

9:40 Jonathan Tennyson[1,2]
[1]Department of Physics and Astronomy, University College London, London WC1E 6BT, UK,
[2] Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary
ELECTRON INITIATED CHEMISTRY

10:20 Yu Liu,[1,2] Timothy W. Schmidt[2] and Terry J. Frankcombe[3]
[1] Shanghai University, Shanghai, China
[2] University of New South Wales, Sydney, Australia
[3] University of New South Wales, Canberra, Australia
THE HITCHIKER'S GUIDE TO THE WAVEFUNCTION

11:00 Session break

11:20-12:40 Session J Chair: Balakrishnan Naduvalath

11:20 Ralph Jaquet
Theoretical Chemistry, University Siegen, 57068 Siegen, Germany
A COMPLETE CONSIDERATION OF NON-ADIABATIC EFFECTS (UP TO ORDER $O(\mu^{-2})$, μ= REDUCED NUCLEAR MASS) IN A TRIATOMIC MOLECULE: INFLUENCE ON THE ROVIBRATIONAL ENERGIES OF H_3^+

12:00 Pablo Gamallo,[1] Alexandre Zanchet,[2] Javier F. Aoiz,[2] and Carlo Petrongolo[3]
1 Departament de Ciència de Materials i Química Física, Universitat, Barcelona, Spain
2 Departamento de Química Física, Universidad Complutense, Madrid, Spain
3 Istituto per Processi Chimico-Fisici, CNR, Pisa, Italy
NON-ADIABATIC QUANTUM DYNAMICS OF THE ELECTRONIC QUENCHING $OH(A^2\Sigma^+) + Kr$

12:40 Lunch break

14:30-16:10 Session K Chair: Alberto García-Vela

14:30 Rupayan Biswas, Dipanshu Kumar, and Upakarasamy Lourderaj
National Insitute of Science Education and Research Bhubaneswar, Odisha, India
ENERGY TRANSFER AND ROTATIONAL RAINBOW OF FORMALDEHYDE SCATTERED FROM SURFACES

15:10 Tibor Nagy, György Lendvay
Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Budapest, Hungary
BEYOND THE NORMAL MODE PICTURE: THE IMPORTANCE OF THE REACTANT'S INTRAMOLECULAR MODE COUPLING IN QUASICLASSICAL TRAJECTORY SIMULATIONS

Wednesday 07. September 2022

15:40 J. Zs. Mezei,[1] G. Fazekas,[2] J. Boffelli,[3] F. Gauchet,[3] M. Ayouz,[4] V. Kokoouline,[5] D. Talbi,[6] K Chakrabart,[7] J. Tennyson,[8] and I. F. Schneider[3]
[1] Institute for Nuclear Research (ATOMKI), Debrecen, Hungary, [2] University of Debrecen, Debrecen, Hungary, [3] LOMC, CNRS University Le Havre Normandy, Le Havre, France
[4] LGPM, CNRS University Paris-Saclay, Gif-sur-Yvette, France, [5] University of Central Florida, Orlando, Florida, USA, [6] LUPM, CNRS University of Montpellier, Montpellier, France, [7]Scottish Church College, Kolkata, India, [8]University College London, London, UK
ELECTRON INDUCED REACTIVITY IN MOLECULAR CATIONS

16:20 Session break

16:40-18:20 Session L Chair: Ralph Jaquet

16:40 Alexandre Zanchet and Octavio Roncero
Instituto de Física Fundamental, CSIC, Madrid, Spain
UNRAVELING THE CRUCIAL ROLE OF SPIN-ORBIT COUPLINGS IN THE REACTIVE COLLISION $S^+ + H_2$

17:40 Tamás Szidarovszky
Institute of Chemistry, ELTE Eötvös Loránd University and MTA-ELTE Complex Chemical Systems Research Group, Pázmány Péter sétány 1/A, H-1117 Budapest, Hungary
SIMULATING THE ROVIBRATIONAL POLARITONS OF H_2O IN INFRARED MICROCAVITIES

18:20 Break

18:30 Dinner

Thursday 08. September 2022.

9:00-11:00 Session M Chair: Dmitri Babikov

9:00 Balakrishnan Naduvalath
Marquette University, Milwaukee, Wisconsin, USA
NON-ADIABATIC AND STEREODYNAMIC EFFECTS IN COLD COLLISIONS

9:40 Domonkos A. Tasi and Gábor Czakó
MTA-SZTE Lendület Computational Reaction Dynamics Research Group, Interdisciplinary Excellence Centre and Department of Physical Chemistry and Materials Science, University of Szeged, Szeged, Hungary
DYNAMICS OF THE OH^- + CH_3F REACTION: THE OXIDE ION SUBSTITUTION

10:00 Session break

10:20-12:00 Session N Chair: George C. Schatz

11:00 Gunnar Nyman
University of Gothenburg, Gothenburg, Sweden
FORMATION OF SMALL MOLECULES IN INTERSTELLAR SPACE

11:40 Uwe Manthe
Theoretische Chemie, Fakultät für Chemie, Universität Bielefeld, Universitätstr. 25, 33615 Bielefeld, Germany
PRODUCT STATE CONTROL AND FAST BARRIER PASSAGE IN POLYATOMIC REACTIONS

11:40 Concluding remarks

12:00 Lunch break

13:00 Boat trip to Tihany

13:30 Boat leaves from Balatonföldvár port

18:00 Boat leaves Tihany port

Friday 09. September 2022.

Dispersal