

Advances in theory of electronic resonances, July 13-17, 2021

Organizers:

Prof. Thomas Jagau, Department of Chemistry, KU Leuven, Belgium

Prof. Anna Krylov, Department of Chemistry, University of Southern California, Los Angeles, USA

Prof. Ksenia Bravaya, Department of Chemistry, Boston University, Boston, USA

The aim of the workshop is to facilitate in-depth discussions of current trends in theoretical description of metastable electronic states and to make connections between theory and experiment. The event brings together people who approach this challenge by various methods ranging from scattering theory to complex absorbing potentials, complex scaling, R-matrix, stabilization techniques, etc. The program will include research presentations and ample discussion time.

ZOOM details:

<https://zoom.us/j/92908120439?pwd=VEVSMUNjRm52bnRPOEFWbjRMZUh1Zz09>

Meeting ID: 929 0812 0439

Passcode: 783804

One tap mobile

+13462487799,,92908120439# US

In-person participants have three different options for displaying their presentation.

1. They can email their presentation to RM1219@telluridescience.org and open it on the room's desktop computer
2. They can put their presentation on a flash drive and load it on to the room's desktop
3. Log into the Zoom meeting with their laptop and share their screen (CRITICAL STEP: they must be muted and have their volume off).

All talks are 30 min + 15 min discussion

Times are given as “Mountain Daylight Time / Central European Daylight Time”

Tuesday, July 13:

SESSION I (Chair: Thomas Jagau)

7:45 am / 3:45 pm Opening remarks

8:00 am / 4:00 pm Lorenz Cederbaum (Heidelberg) “Is an efficient intermolecular energy transfer from vibrations to electronic motion possible?”

8:45 am / 4:45 pm Jimena Gorfinkiel (The Open University) “Use of the R-matrix method for the identification and characterisation of electronic resonances”

9:30 am / 5:30 pm BREAK

SESSION II (Chair: Ksenia Bravaya)

10:00 am / 6:00 pm Anna Krylov (USC) "Dissociative electron attachment via electronic resonances"

10:45 am / 6:45 pm Spiridoula Matsika (Temple) "Comparing different theoretical approaches to describe shape and Feshbach resonances"

11:30 am / 7:30 pm Cate Anstöter (Temple) "Modelling the ultrafast electron attachment dynamics of solvated uracil"

12:15 pm / 8:15 pm END

Wednesday, July 14:

SESSION III (Chair: Jan Verlet)

7:45 am / 3:45 pm Juraj Fedor (Prague) "Resonances in electron-molecule collisions: some recent experimental results"

8:30 am / 4:30 pm Peter Saalfrank (Potsdam) "Resonances and complex potentials in theoretical surface science"

9:15 am / 5:15 pm BREAK

SESSION IV (Chair: Andreas Dreuw)

9:45 am / 5:45 pm Nimrod Moiseyev (Technion) "Electronic and Nuclear resonances by black box calculations from first principles (ab initio)"

10:30 am / 6:30 pm Arik Landau (Technion) TBA

11:15 am / 7:15 pm BREAK

SESSION V (Chair: Ken Jordan)

11:45 am / 7:45 pm Richard Mabbs (Washington U in St. Louis) "Finding Resonances with Photoelectron Angular Distributions - What the Experimentalist Needs to Know"

12:30 pm / 8:30 pm Wojtek Skomorowski (Warsaw) "Autoionizing states in molecules from equation-of-motion coupled-cluster theory combined with Fano-Feshbach ansatz"

1:15 pm / 9:15 pm END

Thursday, July 15:

SESSION VI (Chair: Pierre-François Loos)

7:45 am / 3:45 pm Fernando Martin (Madrid) "Molecular-frame photoelectron angular distributions in the vicinity of Feshbach resonances. The XChem approach"

8:30 am / 4:30 pm Eleonora Luppi (Paris) "New theoretical approaches to study single- and multi-photon ionisation in atoms and molecules"

9:15 am / 5:15 pm BREAK

SESSION VII (Chair: Spiridoula Matsika)

9:45 am / 5:45 pm Ken Jordan (Pittsburgh) "The Stabilization Method Revisited"

10:30 am / 6:30 pm Thomas Jagau (KU Leuven) "Treatment of Molecular Auger Decay by Means of Complex-Variable Coupled-Cluster Methods"

11:15 am / 7:15 pm BREAK

SESSION VIII (Chair: Sylwia Ptasinska)

11:45 am / 7:45 pm Lai-Sheng Wang (Brown) "Probing Dipole-Bound States Using High-Resolution Resonant Photoelectron Imaging of Cryogenically-Cooled Anions"

12:30 pm / 8:30 pm Jan Verlet (Durham) "Effect of solvation on electronic resonances: two sides of a coin"

1:15 pm / 9:15 pm END

Friday, July 16:

SESSION IX (Chair: Jérôme Loreau)

7:45 am / 3:45 pm Pierre-François Loos (Toulouse) "Traditional and Variational Coupled Cluster for Ground and Excited States"

8:30 am / 4:30 pm Andreas Dreuw (Heidelberg) TBA

9:15 am / 5:15 pm BREAK

SESSION X (Chair: Eleonora Luppi)

9:45 am / 5:45 pm Stefanie Gräfe (Jena) "Plasmonic hybrid systems in external light fields: can we achieve sub-nanometer lateral resolution using near-field techniques?"

10:30 am / 6:30 pm Vitali Averbukh (Imperial College London) TBA

11:15 am / 7:15 pm Berny Schlegel (Wayne State) "Simulation of Electron Dynamics in Intense Laser Fields Using Time-Dependent Configuration Interaction"

12:00 pm / 8:00 pm END

Saturday, July 17:

SESSION XI (Chair: Richard Mabbs)

7:45 am / 3:45 pm Jérôme Loreau (KU Leuven) "Resonances in low temperature molecular collisions"

8:30 am / 4:30 pm Thomas Sommerfeld (Southeastern Louisiana) "Resonances of Beryllium trimer dianions"

9:15 am / 5:15 pm BREAK

SESSION XII (Chair: Anna Krylov)

9:45 am / 5:45 pm Sylwia Ptasinska (Notre Dame) "Electron-induced bond dissociation in amides"

10:30 am / 6:30 pm Fabris Kossoski (Toulouse) "Trajectory surface hopping dynamics of electronic resonances"

11:15 am / 7:15 pm Ksenia Bravaya (Boston U) TBA

12:00 pm / 8:00 pm Closing remarks + discussion about future workshops

12:15 pm / 8:15 pm END

Invited Speakers (27 total):

Cate Anstöter (Temple) csanstoter@gmail.com "Modelling the ultrafast electron attachment dynamics of solvated uracil"

Vitali Averbukh (Imperial College London) v.averbukh@imperial.ac.uk TBA

Ksenia Bravaya (Boston U) kbravaya@gmail.com TBA

Lorenz Cederbaum (Heidelberg) lorenz.cederbaum@pci.uni-heidelberg.de "Is an efficient intermolecular energy transfer from vibrations to electronic motion possible?"

Andreas Dreuw (Heidelberg) dreuw@iwr.uni-heidelberg.de TBA

Juraj Fedor (Prague) juraj.fedor@jh-inst.cas.cz "Resonances in electron-molecule collisions: some recent experimental results"

Jimena Gorfinkiel (The Open University) jimena.gorfinkiel@open.ac.uk "Use of the R-matrix method for the identification and characterisation of electronic resonances"

Stefanie Gräfe (Jena) s.graefe@uni-jena.de "Plasmonic hybrid systems in external light fields: can we achieve sub-nanometer lateral resolution using near-field techniques?"

Thomas Jagau (KU Leuven) thomas.jagau@kuleuven.be "Treatment of Molecular Auger Decay by Means of Complex-Variable Coupled-Cluster Methods"

Ken Jordan (Pittsburgh) jordan@pitt.edu "The Stabilization Method Revisited"

Fabris Kossoski (Toulouse) fkossoski@irsamc.ups-tlse.fr "Trajectory surface hopping dynamics of electronic resonances"

Anna Krylov (USC) krylov@usc.edu "Dissociative electron attachment via electronic resonances"

Arik Landau (Technion) arik.landau@technion.ac.il TBA

Pierre-François Loos (Toulouse) pierrefrancois.loos@gmail.com “Traditional and Variational Coupled Cluster for Ground and Excited States”

Jérôme Loreau (KU Leuven) jerome.loreau@kuleuven.be “Resonances in low temperature molecular collisions”

Eleonora Luppi (Paris) eleonora.luppi@upmc.fr “New theoretical approaches to study single- and multi-photon ionisation in atoms and molecules”

Richard Mabbs (Washington U in St. Louis) mabbs@wustl.edu “Finding Resonances with Photoelectron Angular Distributions - What the Experimentalist Needs to Know”

Fernando Martin (Madrid) fernando.martin@uam.es “Molecular-frame photoelectron angular distributions in the vicinity of Feshbach resonances. The XChem approach”

Spiridoula Matsika (Temple) smatsika@temple.edu “Comparing different theoretical approaches to describe shape and Feshbach resonances”

Nimrod Moiseyev (Technion) nimrod@technion.ac.il “Electronic and Nuclear resonances by black box calculations from first principles (ab initio)”

Sylwia Ptasinska (Notre Dame) Sylwia.Ptasinska.1@nd.edu “Electron-induced bond dissociation in amides”

Peter Saalfrank (Potsdam) peter.saalfrank@uni-potsdam.de “Resonances and complex potentials in theoretical surface science”

Berny Schlegel (Wayne State) hbs@chem.wayne.edu “Simulation of Electron Dynamics in Intense Laser Fields Using Time-Dependent Configuration Interaction”

Wojciech Skomorowski (Warsaw) wojciech.skomorowski@gmail.com “Autoionizing states in molecules from equation-of-motion coupled-cluster theory combined with Fano-Feshbach ansatz”

Thomas Sommerfeld (Southeastern Louisiana) Thomas.Sommerfeld@southeastern.edu “Resonances of Beryllium trimer dianions”

Jan Verlet (Durham) j.r.r.verlet@durham.ac.uk “Effect of solvation on electronic resonances: two sides of a coin”

Lai-Sheng Wang (Brown) lai-sheng_wang@brown.edu “Probing Dipole-Bound States Using High-Resolution Resonant Photoelectron Imaging of Cryogenically-Cooled Anions”