

Title: “Advances in theory of electronic resonances”

Organizers:

Prof. Anna Krylov, Department of Chemistry, University of Southern California, Los Angeles, USA
Prof. Ksenia Bravaya, Department of Chemistry, Boston University, Boston, USA
Dr. Thomas Jagau, Department of Chemistry, University of Munich, Munich, Germany

Location: Telluride Elementary School, 477 West Columbia Ave Telluride CO 81435

TSRC Hosts: Mark Kozak (970) 708-4426, Kristen Redd (970) 708-0827

Time: July 17-21, 2017

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 several introductory lectures as well as research presentations and ample discussion time.

Schedule: All talks are 30 min + 15 min discussion

Sunday, July 16: 6:00-9:00 pm

Meet and greet TSRC reception at [the Phoenix Bean](#) on Main street (221 W. Colorado Ave).

A representative from TSRC will be there 6-8 pm to hand out badges, welcome folks to town, and answer your questions. You will need your badge for the drink specials. Guests and family members are welcome.

Monday, July 17:

7:30 BREAKFAST

MORNING SESSION (Chair: Anna Krylov)

8:00 Opening remarks

8:15 Nimrod Moiseyev (Technion) “New theory for new technology: cross sections for cold collision experiments from ab-initio CPESs (complex potential energy surfaces)”

9:00 Matthias Ernzerhof (Montreal) “Resonances in systems consisting of quantized photons and electrons”

9:45 BREAK

10:15 Spiridoula Matsika (Temple) “Resonances and dissociative electron attachment in uracil using stabilization methods“

11:00 Mike Falcetta (Grove City College) “Application of the Stabilization Method via exponent scaling to resonances in model, atomic and molecular systems“

11:45 END

EVENING SESSION (Chair: Richard Mabbs)

7:00 Andrei Sanov (U Arizona) "Photoelectron imaging spectroscopy of weakly bound anions and transient neutral molecules"

7:45 Antonia Karamatskou (CFEL Hamburg) "Uncovering hidden resonances through multiphoton ionization"

8:30 END

Tuesday, July 18:

7:30 BREAKFAST

AFTERNOON SESSION (Chair: Andreas Dreuw)

2:00 Anna Krylov (USC) "Not all dipoles are created equal: On the existence of dipole-bound and dipole-stabilized states in open- and closed-shell species"

2:45 Wojciech Skomorowski (USC) "Theoretical predictions of resonances and bound states in cyanopolyne anions"

3:30 BREAK

4:00 Thomas Jagau (Munich) "Coupled-cluster methods for shape and Feshbach resonances"

4:45 END

6:00-7:00 Town talk

Wednesday, July 19:

7:30 BREAKFAST

AFTERNOON SESSION (Chair: Matthias Ernzerhof)

2:00 Richard Mabbs (Washington U) "Probing vibrational modes of unstable anion states and channel specific autodetachment"

2:45 Sylwia Ptasinska (Notre Dame) "Direct observation of neutral radicals from a dissociative electron attachment process"

3:30 BREAK

4:00 Ken Jordan (Pittsburgh) "Non-valence correlation bound anions: Connections with resonances and virtual states"

4:45 Debarati Bhattacharya (Technion) "Ab-initio complex potential energy surfaces for ultracold atom-molecule collision"

5:30 END and **take workshop group picture**

6:00-9:00 TSRC picknick

Thursday, July 20:

7:30 BREAKFAST

AFTERNOON SESSION (Chair: Nimrod Moiseyev)

2:00 Armin Scrinzi (Munich) "Electronic structure and photo-emission in strong fields: irECS, haCC, and tSurff"

2:45 Kirill Gokhberg (Heidelberg) "Electron transfer processes and neutralization of multiply charged ions in clusters"

3:30 BREAK

4:00 Ksenia Bravaya (Boston U) "Multireference perturbation theory for metastable electronic states"

4:45 Andreas Dreuw (Heidelberg) "Lifetimes of decaying states using ADC"

5:30 END

EVENING SESSION (Chair: Thomas Jagau)

7:00 Alec White (Berkeley) "Methods for electronic resonances: Applications to complex potential energy surfaces"

7:45 Ashish Kumar Gupta (IIT Guwahati) "Application of modified smooth exterior scaling method for calculation of Auger resonance in Be using zeroth-order and second-order electron propagator"

8:30 END

Friday, July 21:

7:30 BREAKFAST

MORNING SESSION (Chair: Ksenia Bravaya)

8:00 Danny Yeager (Texas A&M) "Studies with the complex scaled multiconfigurational spin-tensor electron propagator method (CMCSTEP) and a few other things"

8:45 Arik Landau (Technion) "Basic and applicable aspects in analytical continuation (from stabilization graphs) schemes for electronic resonance states"

9:30 BREAK

10:00 Vitaly Rassolov (U South Carolina) tba

10:45 Closing remarks and farewell, discussion about future workshops

END

Participants (22 total):

Debarati Bhattacharya (Technion) debarati01@gmail.com (Moiseyev) "Ab-initio complex potential energy surfaces for ultracold atom-molecule collision"

Ksenia Bravaya (BU) kbravaya@gmail.com "Multireference perturbation theory for metastable electronic states"

Andreas Dreuw (Heidelberg) dreuw@uni-heidelberg.de "Lifetimes of decaying states using ADC"

Matthias Ernzerhof (Montreal) matthias.Ernzerhof@UMontreal.ca "Resonances in systems consisting of quantized photons and electrons"

Mike Falcetta (Grove City College) mffalcetta@gcc.edu "Application of the Stabilization Method via exponent scaling to resonances in model, atomic and molecular systems"

Kirill Gokhberg (Heidelberg) Kirill.Gokhberg@tc.pci.uni-heidelberg.de "Electron transfer processes and neutralization of multiply charged ions in clusters"

Ashish Kumar Gupta (IIT Guwahati) gupta@iitg.ernet.in "Application of modified smooth exterior scaling method for calculation of Auger resonance in Be using zeroth-order and second-order electron propagator"

Thomas Jagau (Munich) thjapc@cup.uni-muenchen.de “Coupled-cluster methods for shape and Feshbach resonances”

Ken Jordan (Pittsburgh) jordan@pitt.edu “Non-valence correlation bound anions: Connections with resonances and virtual states”

Antonia Karamatskou (CFEL Hamburg) antonia.karamatskou@cfel.de “Uncovering hidden resonances through multiphoton ionization”

Anna Krylov (USC) krylov@usc.edu “Not all dipoles are created equal: On the existence of dipole-bound and dipole-stabilized states in open- and closed-shell species”

Arik Landau (Technion) arik.landau@gmail.com “Basic and applicable aspects in analytical continuation (from stabilization graphs) schemes for electronic resonance states”

Richard Mabbs (Washington Univ) mabbs@wustl.edu “Probing vibrational modes of unstable anion states and channel specific autodetachment”

Spiridoula Matsika (Temple) smatsika@temple.edu “Resonances and dissociative electron attachment in uracil using stabilization methods”

Nimrod Moiseyev (Technion) nimrod@techunix.technion.ac.il “New theory for new technology: cross sections for cold collision experiments from ab-initio CPESs (complex potential energy surfaces)”

Sylwia Ptasinka (Notre Dame) sptasins@nd.edu “Direct observation of neutral radicals from a dissociative electron attachment process”

Vitaly Rassolov (U South Carolina) RASSOLOV@mailbox.sc.edu

Andrei Sanov (U Arizona) sanov@email.arizona.edu “Photoelectron imaging spectroscopy of weakly bound anions and transient neutral molecules”

Armin Scrinzi (Munich) armin.scrinzi@physik.uni-muenchen.de “Electronic structure and photo-emission in strong fields: irECS, haCC, and tSurff”

Wojciech Skomorowski (USC) wojciech.skomorowski@gmail.com “Theoretical predictions of resonances and bound states in cyanopolyne anions”

Alec White (Berkeley) whiteaf@berkeley.edu “Methods for electronic resonances: Applications to complex potential energy surfaces”

Danny Yeager (Texas A&M) yeager@chem.tamu.edu “Studies with the complex scaled multiconfigurational spin-tensor electron propagator method (CMCSTEP) and a few other things”