

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, University of Munich, Munich, Germany

Location: Telluride Intermediate School, 725 West Colorado Ave, Telluride CO, 81435

TSRC Hosts: Mark Kozak (970) 708-4426

Time: July 22-26, 2019

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.

Schedule: All talks are 40 min + 15 min discussion

Sunday, July 21:

5:00 - 6:30 TSRC Meet and Greet event at [Oak](#) located at the base of the gondola at [250 W San Juan Avenue \(Gus's Way\)](#)

Monday, July 22:

7:30 BREAKFAST

MORNING SESSION (Chair: Anna Krylov)

8:00 Opening remarks

8:15 Jan Verlet (Durham) “Probing electron impact resonances with photons”

9:10 Michael Allan (Fribourg) “Two-dimensional electron-energy loss spectra reveal nuclear dynamics of negative ion resonances”

10:05 BREAK

10:35 Thomas Jagau (Munich) “Two methodological developments for electronic resonances: Analytic gradients and a resolution-of-the-identity approximation”

11:30 Patrick Norman (KTH Stockholm) “VeloxChem: a highly modular Python-driven software initiative for spectroscopic properties of complex molecular systems”

12:25 END AND WORKSHOP GROUP PICTURE

AFTERNOON SESSION (Chair: Spiridoula Matsika)

2:30 Anna Krylov (USC Los Angeles) “Orbital concepts in non-Hermitian quantum chemistry”

3:25 Wojciech Skomorowski (USC Los Angeles) “New insights into specific Fano-Feshbach autoionizing states from EOM-CCSD method and two-body Dyson matrices”

4:20 BREAK

4:50 Lai-Sheng Wang (Brown U) "Resonant Photoelectron Spectroscopy of Cold Anions via Dipole-Bound Excited States"

5:45 END

Tuesday, July 23:

7:30 BREAKFAST

AFTERNOON SESSION (Chair: Patrick Norman)

2:00 Spiridoula Matsika (Temple U) TBA

2:55 Adrian Dempwolff (Heidelberg) "Resonances with ADC"

3:50 BREAK

4:20 Ksenia Bravaya (Boston U) TBA

5:15 END

6:30 "**2019 R. STEPHEN BERRY LECTURE**, Lynn Loo (Princeton U): "Getting to Zero: How fast can we reduce carbon emissions?"

Location: Telluride Conference Center in Mountain Village

Admission is free, Cash Bar starts at 6:00

Wednesday, July 24:

7:30 BREAKFAST

AFTERNOON SESSION (Chair: Michael Allan)

2:00 Ken Jordan (Pittsburgh) "Non-valence Anions: Bound States and Resonances"

2:55 Arailym Kairalapova (Pittsburgh) "Non-valence Anion States of (NaCl)₂"

3:30 BREAK

4:00 Jesús González-Vázquez (Madrid) "The XCHEM method: A Gaussian Bspline approach for electronic continuum"

4:55 END

6:00 - 8:00 TSRC picnic

Location: Telluride Intermediate School, 725 West Colorado Ave, Telluride CO, 81435

Thursday, July 25:

7:30 BREAKFAST

AFTERNOON SESSION (Chair: Ken Jordan)

2:00 Mi Kyung Lee (Wayne State U) TBA

2:55 Roman Curik (J. Heyrovsky Institute, Prague) "Resonances and nuclear dynamics of polyatomic molecules"

3:50 BREAK

4:20 Richard Mabbs (Washington U) "Photoelectron Angular Distributions as Indicators of Resonances"

5:15 END

Friday, July 26:

7:30 BREAKFAST

MORNING SESSION (Chair: Ksenia Bravaya)

8:00 Matthias Ernzerhof (Montreal) "Relating non-Hermitian quantum mechanics, complex energies, and exceptional points to open systems"

8:55 Martin Cizek (Charles U, Prague) "Towards implementation of projection-operator description of resonances in R-matrix software"

9:50 BREAK

10:20 Florian Hampe (Mainz) TBA

11:15 Closing remarks and farewell, discussion about future workshops

11:30 END

Participants (19 total):

Michael Allan (Fribourg) michael.allan@bluewin.ch "Two-dimensional electron-energy loss spectra reveal nuclear dynamics of negative ion resonances"

Ksenia Bravaya (Boston U) kbravaya@gmail.com

Martin Cizek (Charles U, Prague) cizek@mbox.troja.mff.cuni.cz "Towards implementation of projection-operator description of resonances in R-matrix software"

Roman Curik (J. Heyrovsky Institute, Prague) roman.curik@jh-inst.cas.cz "Resonances and nuclear dynamics of polyatomic molecules"

Adrian Dempwolff (Heidelberg) adrian.dempwolff@iwr.uni-heidelberg.de "Resonances with ADC"

Matthias Ernzerhof (Montreal) Matthias.Ernzerhof@umontreal.ca "Relating non-Hermitian quantum mechanics, complex energies, and exceptional points to open systems"

Jesús González-Vázquez (Madrid) jesus.gonzalezv@uam.es "The XCHEM method: A Gaussian Bspline approach for electronic continuum"

Florian Hampe (Mainz) hampe@uni-mainz.de

Thomas Jagau (Munich) th.jagau@lmu.de "Two methodological developments for electronic resonances: Analytic gradients and a resolution-of-the-identity approximation"

Ken Jordan (Pittsburgh) jordan@pitt.edu "Non-valence Anions: Bound States and Resonances"

Arailym Kairalapova (Pittsburgh) "Non-valence Anion States of (NaCl)₂"

Anna Krylov (USC Los Angeles) krylov@usc.edu “Orbital concepts in non-Hermitian quantum chemistry”

Mi Kyung Lee (Wayne State U)

Richard Mabbs (Washington U) mabbs@wustl.edu “Photoelectron Angular Distributions as Indicators of Resonances”

Spiridoula Matsika (Temple U) smatsika@temple.edu

Patrick Norman (KTH Stockholm) panor@kth.se “VeloxChem: a highly modular Python-driven software initiative for spectroscopic properties of complex molecular systems”

Wojciech Skomorowski (USC Los Angeles) wojciech.skomorowski@gmail.com “New insights into specific Fano-Feshbach autoionizing states from EOM-CCSD method and two-body Dyson matrices”

Jan Verlet (Durham) j.r.r.verlet@durham.ac.uk “Probing electron impact resonances with photons”

Lai-Sheng Wang (Brown U) Lai-Sheng_Wang@brown.edu “Resonant Photoelectron Spectroscopy of Cold Anions via Dipole-Bound Excited States”