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

Location: Telluride Intermediate School, 721 West Colorado Ave Telluride CO 81435
TSRC Hosts: Mark Kozak (970) 708-4426

Time: July 22-26, 2024

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 30 min + 15 min discussion

Sunday, July 21:
5:00 - 6:30 All-Telluride Science Meet and Greet at Alibi – 157 S. Fir Street

Monday, July 22:
7:30 BREAKFAST

MORNING SESSION (Chair: Anna Krylov)
8:00 Opening remarks
8:15 Lai-Sheng Wang (Brown U) "Probing vibrational Feshbach resonances and shape resonances of cryogenically-cooled PAH anions"
9:00 Juraj Fedor (J. Heyrovsky Institute, Prague) "Resonances in electron-molecule collisions: some recent experimental results"
9:45 BREAK
10:15 Thomas Jagau (KU Leuven) "Modeling dissociative electron attachment with complex-variable methods"
11:00 Wojciech Skomorowski (U of Warsaw) "Benchmarking Fano-Feshbach calculations of autoionization widths based on EOM-CCSD wave function"
11:45 END AND WORKSHOP GROUP PICTURE

AFTERNOON SESSION (Chair: Spiridoula Matsika)
2:00 Anna Krylov (USC Los Angeles) TBA
2:45 Andrei Sanov (U of Arizona) “When chemistry isn’t real: The temporary anions of unsaturated polycyclic organics in charge-transfer cluster photodetachment”
3:30 BREAK
4:00 Kenneth Jordan (U of Pittsburgh) “Extracting partial widths for temporary anion resonance”
4.45 Stephen Slimak (U of Pittsburgh) “Characterization of 2p1h resonances in polyaromatic hydrocarbons”
5:30 END

Tuesday, July 23:
7:30 BREAKFAST

AFTERNOON SESSION (Chair: Ksenia Bravaya)
2:00 Sonia Coriani (Technical U of Denmark) “Simulating photoabsorption, photoionisation and autoionisation processes by correlated methods”
2:45 Florian Matz (KU Leuven) “Theoretical description of Auger decay with complex-variable methods”
3:30 BREAK
4:00 Spiridoula Matsika (Temple U) “Metastable anions in gas and condensed phases”
4:45 END

6:30 Telluride Town Talk: “Clean Energy’s Reliance on Dirty Magnets:The Source and a Solution”; Speaker: Peter Ladwig (VP of Nanoparticle Development Niron Magnetics).
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: Ken Jordan)
2:00 Ksenia Bravaya (Boston U) “Projected CAP methods for shape and Feshbach resonances”
2:45 Matthieu Génévriez (UC Louvain) “Double Rydberg states: Theory of two-electron resonances far from the nucleus”
3:30 BREAK
4:00 Elke Fasshauer (University of Tübingen) TBA
4:45 END

5:30 - TSRC picnic
Location: Telluride Intermediate School, 725 West Colorado Ave, Telluride CO, 81435

Thursday, July 25:
7:30 BREAKFAST

AFTERNOON SESSION (Chair: Sonia Coriani)
2:00 Ilya Fabrikant (U of Nebraska – Lincoln) "Resonances in electron and positronium scattering by molecules"
2:45 Martin Cizek (Institute of Theoretical Physics, Prague) “Vibronic coupling of electronic resonances in polyatomic molecules”
3:30 BREAK
4:00 Soubhik Mondal (Boston U) “Nuclear dynamics in metastable electronic states”
4.45 Jan Dvorak (LBNL) “Effect of autoionizing states on one-color two-photon ionization dynamics of O_2 molecule”
5.30 END

Friday, July 26:
7:30 BREAKFAST

MORNING SESSION (Chair: Thomas Jagau)
8:00 Michal Tomza (U of Warsaw) “Quantum resonances in ultracold atom-ion and atom-molecule collisions”
8:45 Richard Mabbs (Washington U in St. Luis) “"Alkyl Halide Cluster Anion Photoelectron Angular Distributions: A Career Long Puzzle (or Don't Forget the Nuclear Degrees of Freedom When Considering Excited Anion States!)"
9:30 BREAK
10:00 Closing remarks and farewell, discussion about future workshops
10.30 END