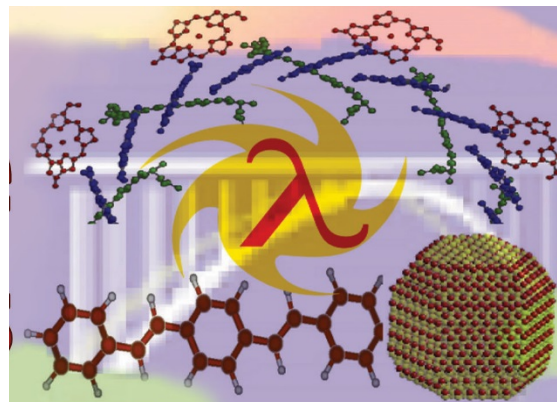


Updated 05/28/2023

## Conference Program



*The 10<sup>th</sup> International Conference on*

# **EXCITED STATE PROCESSES IN ELECTRONIC AND BIO NANOMATERIALS**

## **ESP-2023**

**June 5 – June 8, 2023**

**Santa Fe, New Mexico, USA**

<http://cnls.lanl.gov/esp2023>

*The conference is sponsored by Center for Nonlinear Studies (CNLS); Center for Integrated Nanotechnologies (CINT); Theoretical, Chemistry and Materials Physics and Applications at Los Alamos National Laboratory; and supported by the U.S. Department of Energy.*

*Conference organizers:* Sergei Tretiak, Tammie (Nelson) Gibson

*Conference e-mail:* [serg@lanl.gov](mailto:serg@lanl.gov), [tammien@lanl.gov](mailto:tammien@lanl.gov)

*The Advisory Committee:* Enrique Batista, Victor Klimov, Amanda Neukirch, Wanyi Nie, Andrei Piryatinski, Valy Vardeny

*Conference coordinator:* Leah Bulnes, [cnls-conferences@lanl.gov](mailto:cnls-conferences@lanl.gov)

*Location:* Hotel Santa Fe, 1501 Paseo de Peralta

Santa Fe, New Mexico 87501

(855) 825-9876 (oral presentations, poster sessions, banquet)



invited talks = 35 min (30 min + 5 min questions)

contributed talks = 20 min (15 min + 5 min questions)

coffee break w/ snacks = 20 min

lunch on your own = 1.5 hr

poster session w/ snacks & cash bar = 2 hr

| Monday, June 5                       | Tuesday, June 6                       | Wednesday, June 7                  | Thursday, June 8                |
|--------------------------------------|---------------------------------------|------------------------------------|---------------------------------|
| <b>Welcome</b><br>8:25-9:00          | <b>TROISI</b><br>8:25-9:00            | <b>VARDENY</b><br>8:25-9:00        | <b>GROSS</b><br>8:25-9:00       |
| <b>SCHOLES</b><br>9:00-9:35          | <b>STINGELIN</b><br>9:00-9:35         | <b>KAMBHAMPATI</b><br>9:00-9:35    | <b>MAZUMDAR</b><br>9:00-9:35    |
| <b>MCCUSKER</b><br>9:35-10:10        | <b>DA COMO</b><br>9:35-10:10          | <b>NIE</b><br>9:35-10:10           | <b>SFEIR</b><br>9:35-10:10      |
| <b>Coffee</b><br>10:10-10:30         | <b>Coffee</b><br>10:10-10:30          | <b>Coffee</b><br>10:10-10:30       | <b>Coffee</b><br>10:10-10:30    |
| <b>FREIXAS</b><br>10:30-10:50        | <b>LIVACHE</b><br>10:30-10:50         | <b>HE</b><br>10:30-10:50           | <b>PETERSON</b><br>10:30-10:50  |
| <b>NEATON</b><br>10:50-11:25         | <b>MARDER</b><br>10:50-11:25          | <b>PAO</b><br>10:50-11:25          | <b>DEXHEIMER</b><br>10:50-11:25 |
| <b>ONOE</b><br>11:25-12:00           | <b>JONSSON</b><br>11:25-12:00         | <b>NIENHAUS</b><br>11:25-12:00     | <b>LIENAU</b><br>11:25-12:00    |
| <b>Lunch</b><br>12:00-1:30           | <b>Lunch</b><br>12:00-1:30            | <b>Lunch</b><br>12:00-1:30         | <b>Lunch</b><br>12:00-1:30      |
| <b>CHEN</b><br>1:30-2:05             | <b>CROOKER</b><br>1:30-2:05           | <b>SON</b><br>1:30-2:05            | <b>TSAI</b><br>1:30-2:05        |
| <b>BEARD</b><br>2:05-2:40            | <b>KRYLOV</b><br>2:05-2:40            | <b>BITTNER</b><br>2:05-2:40        | <b>NEUKIRCH</b><br>2:05-2:40    |
| <b>CERULLO</b><br>2:40-3:15          | <b>FURCHE</b><br>2:40-3:15            | <b>SILVA</b><br>2:40-3:15          | <b>AHN</b><br>2:40-3:15         |
| <b>Coffee</b><br>3:15-3:35           | <b>Coffee</b><br>3:15-3:35            | <b>Coffee</b><br>3:15-3:35         | <b>Coffee</b><br>3:15-3:35      |
| <b>MUKAMEL</b><br>3:35-4:10          | <b>TANIMURA</b><br>3:35-4:10          | <b>HTOON</b><br>3:35-4:10          | <b>BRADFORTH</b><br>3:35-4:10   |
| <b>GARAVELLI</b><br>4:10-4:45        | <b>VANMAEKELBERGH</b><br>4:10-4:45    | <b>COTLET</b><br>4:10-4:45         | <b>ZWIER</b><br>4:10-4:45       |
| <b>GOVIND</b><br>4:45-5:20           | <b>J-K WANG</b><br>4:45-5:20          | <b>SHARIFZADEH</b><br>4:45-5:20    | <b>COROPCEANU</b><br>4:45-5:20  |
|                                      |                                       |                                    | <b>Closing</b><br>5:20-5:30     |
| <b>Poster Session I</b><br>7:00-9:00 | <b>Poster Session II</b><br>7:00-9:00 | <b>Banquet Dinner</b><br>7:00-9:00 |                                 |

## Monday, June 5

**08:25am – 09:00am**      **Welcome** (Irene Qualters, Laura Stonehill, Chris Fryer)

### Morning Session:

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Session chair: Tammie (Nelson) Gibson (LANL)

**09:00am – 09:35am**      **Greg Scholes** (Princeton University)

*"A Superposition of Chemical Reactions"*

**09:35am – 10:10am**      **James McCusker** (Michigan State University)

*"Using Coherence to Probe Excited-state Reaction Dynamics in Transition Metal-based Chromophores"*

**10:10am – 10:30am**      **Break**

Session chair: Jen Hollingsworth (LANL)

**10:30am – 10:50am**      **Victor Freixas** (UC Irvine)

*"Monitoring Quantum Coherences with TRUECARS X-Ray Raman Signals"*

**10:50am – 11:25am**      **Jeff Neaton** (UC Berkeley)

*"Phonon-driven Screening, Scattering, and Dissociation of Excitons in Inorganic and Molecular Semiconductors from First Principles"*

**11:25am – 12:00pm**      **Jun Onoe** (Nagoya University)

*"Recycling of Precious Metals using Nanospace Materials"*

**12:00pm – 1:30pm**      **Lunch**

### Afternoon Session:

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Session chair: Travis Jones (LANL)

**01:30pm – 02:05pm**      **Guanhua Chen** (Hong Kong University)

*"Coherent Charge Transport Across a Donor-Acceptor Interface Mediated by Vibronic Couplings"*

**02:05pm – 02:40pm**      **Matt Beard** (NREL)

*"Controlling Spin and Light at Room Temperature in Lead-Halide Inspired Hybrid Semiconductors"*

**02:40pm – 03:15pm**      **Giulio Cerullo** (Politecnico di Milano)

*"Real-time Observation of Conical Intersections in Biomolecules"*

**03:15pm – 03:35pm**      **Break**

Session chair: Avadh Saxena (LANL)

**03:35pm – 04:10pm**      **Shaul Mukamel** (UC Irvine)

*"Probing Conical Intersection Dynamics by Attosecond X-Ray Pulses"*

**04:10pm – 04:45pm**      **Marco Garavelli** (University of Bologna)

*"Photoinduced Ultrafast Energy Transfer and its Transient Spectral Signals by Multidimensional Quantum Dynamics: The Paradigmatic Case of the NADH Dimer"*

**04:45pm – 05:20pm**      **Niri Govind** (Pacific Northwest National Lab)

*"Explorations in Ultrafast Dynamics and X-Ray Spectroscopies"*

**07:00pm**      **Poster Session I**

## Tuesday, June 6

### Morning Session:

---

Session chair: Alex White (LANL)

**08:25am – 09:00am**      **Alessandro Troisi**      (University of Liverpool)

*"Structure-property Relations in Excitons from High-throughput Virtual Screening"*

**09:00am – 09:35am**      **Natalie Stingelin**      (Georgia Tech)

*"Can We Correlate the Nature of Electronic Disorder to Structural Dynamics in Polymer Semiconductors?"*

**09:35am – 10:10am**      **Enrico Da Como**      (University of Bath)

*"Excited States in Charge Density Wave Metal Dichalcogenides Probes in Time and Momentum Space"*

**10:10am – 10:30am**      **Break**

Session chair: Ivana Gonzales (LANL)

**10:30am – 10:50am**      **Clément Livache**      (Los Alamos National Lab)

*"Ultrafast Spin-Exchange Auger Recombination and Carrier Multiplication in Manganese-Doped Colloidal Quantum Dots"*

**10:50am – 11:25am**      **Seth Marder**      (Georgia Tech)

*"Electronic and Optical Properties of Organic Semiconductor/Dopant Systems"*

**11:25am – 12:00pm**      **Hannes Jonsson**      (University of Iceland)

*"Calculations of Excited States by Converging on Saddle Points Using Generalized Mode Following"*

**12:00pm – 1:30pm**      **Lunch**

### Afternoon Session:

---

Session chair: Victor Klimov (LANL)

**01:30pm – 02:05pm**      **Scott Crooker**      (Los Alamos National Lab)

*"6-Particle and 8-Particle Excited States in Monolayer Semiconductors"*

**02:05pm – 02:40pm**      **Anna Krylov**      (U. Southern California)

*"Spin-forbidden Processes and Molecular Magnetism: Theory and Applications"*

**02:40pm – 03:15pm**      **Filipp Furche**      (UC Irvine)

*"Instabilities in Time-Dependent Mean Field Theories"*

**03:15pm – 03:35pm**      **Break**

Session chair: Galen Craven (LANL)

**03:35pm – 04:10pm**      **Yoshitaka Tanimura**      (University of Kyoto)

*"Numerically "Exact" Simulations of Quantum Thermodynamic Machines: Thermodynamic Work Diagrams"*

**04:10pm – 04:45pm**      **Daniel Vanmaekelbergh**      (University of Utrecht)

*"High-energy Excitations in Layered (Topological) Semiconductors. The Case of Colloidal Bi<sub>2</sub>Se<sub>3</sub> Platelets"*

**04:45pm – 05:20pm**      **Juen-Kai Wang**      (NTU, Taipei)

*"Enhancement Factor and Continuum Background of Surface-enhanced Raman Scattering"*

**07:00pm**      **Poster Session II**

## Wednesday, June 7

### Morning Session:

---

Session chair: Jianxin Zhu (LANL)

**08:25am – 09:00am**                      **Valy Vardeny**                      (University of Utah)

*"Optical Probes of the Rashba Splitting in 2D Hybrid Organic Inorganic Perovskites"*

**09:00am – 09:35am**                      **Patanjali Kambhampati**                      (McGill University)

*"Resolving the Spectral Dynamics of Excitonic Complexes in Perovskite Nanocrystals via Time-resolved Photoluminescence Spectroscopy"*

**09:35am – 10:10am**                      **Wanyi Nie**                      (Los Alamos National Lab)

*"Photo Conduction Gain of Perovskite Photo-diode and Hetero-structured Detectors"*

**10:10am – 10:30am**                      **Break**

Session chair: Roxanne Tutchton (LANL)

**10:30am – 10:50am**                      **Sheng He**                      (Emory University)

*"Electron Trapping Prolongs the Lifetime of Charge-Separated States in 2D Perovskite Nanoplatelet-Hole Acceptor Complexes"*

**10:50am – 11:25am**                      **Chung-Wei Pao**                      (Academia Sinica, Taiwan)

*"Mapping the Microstructure of Complex Perovskite Materials Using Machine Learning-based Energy Models"*

**11:25am – 12:00pm**                      **Lea Nienhaus**                      (Florida State University)

*"Sensational Sensitization: Triplet Generation at the Perovskite/Organic Interface"*

**12:00pm – 1:30pm**                      **Lunch**

### Afternoon Session:

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Session chair: Andrei Piryatinski (LANL)

**01:30pm – 02:05pm**                      **Dong Hee Son**                      (Texas A&M)

*"Photoemission of Auger-upconverted Hot Electrons from Mn-doped Perovskite Nanocrystals via Weak CW Visible Excitation"*

**02:05pm – 02:40pm**                      **Eric Bittner**                      (University of Houston)

*"Looking Under the Hood and Unraveling Dark Processes in Excitonic Systems"*

**02:40pm – 03:15pm**                      **Carlos Silva**                      (Georgia Tech)

*"Many-body Exciton Dynamics in Ruddelsden-Popper Metal Halides"*

**03:15pm – 03:35pm**                      **Break**

Session chair: Kipton Barros (LANL)

**03:35pm – 04:10pm**                      **Han Htoon**                      (Los Alamos National Lab)

*"Controlling Polarization of 2D Quantum Emitters with Proximity Effect"*

**04:10pm – 04:45pm**                      **Mircea Cotlet**                      (Brookhaven National Lab)

*"Charge Transfer at Interfaces of Mixed Dimensional Van der Waals Heterostructures"*

**04:45pm – 05:20pm**                      **Sahar Sharifzadeh**                      (Boston University)

*"Computational Understanding of Internal Energy Conversion Dynamics within Stacked Organic Chromophores"*

**07:00pm**                      **Banquet**

**Thursday, June 8**

**Morning Session:**

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Session chair: Nick Lubbers (LANL)

- 08:25am – 09:00am**      **Hardy Gross**      (Hebrew U. of Jerusalem)  
*"Mechanisms of Electronic Decoherence"*
- 09:00am – 09:35am**      **Sumit Mazumdar**      (University of Arizona)  
*"Theoretical Route to Weakly Bound Triplet-Triplet Multiexcitons in Intramolecular Singlet Fission Chromophores"*
- 09:35am – 10:10am**      **Mathew Sfeir**      (CUNY)  
*"Quantum Interference Effects on the Multiexciton Dynamics of Singlet Fission Chromophores"*
- 10:10am – 10:30am**      **Break**

Session chair: Ben Nebgen (LANL)

- 10:30am – 10:50am**      **Elizabeth Peterson**      (Los Alamos National Lab)  
*"Self-energy Corrected Calculations of the Dielectric Function for Light Dark Matter Detection via Electronic Excitation"*
- 10:50am – 11:25am**      **Susan Dexheimer**      (Washington State University)  
*"Formation and Evolution of Nonlinear Excitations in Structurally Tunable Low Dimensional Materials"*
- 11:25am – 12:00pm**      **Christoph Lienau**      (University of Oldenburg)  
*"Strong Coupling, Rabi Oscillations and Many-body Excitations in Exciton-Plasmon System: What Can We Learn from 2D Spectroscopy?"*
- 12:00pm – 1:30pm**      **Lunch**

**Afternoon Session:**

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Session chair: Richard Messerly (LANL)

- 01:30pm – 02:05pm**      **Dave Tsai**      (UC Berkeley)  
*"Improving the Perovskite LEDs Stability by Building Perovskite Heterostructures"*
- 02:05pm – 02:40pm**      **Amanda Neukirch**      (Los Alamos National Lab)  
*"Computational Modeling for the Development of Chiral Quantum Systems"*
- 02:40pm – 03:15pm**      **Namyoun Ahn**      (Los Alamos National Lab)  
*"Colloidal Quantum Dot Laser Diodes: Three Decades in the Making"*
- 03:15pm – 03:35pm**      **Break**

Session chair: Brendan Gifford (LANL)

- 03:35pm – 04:10pm**      **Stephen Bradforth**      (U. Southern California)  
*"Designing and Characterizing Photosensitizers for Solar Fuel Production"*
- 04:10pm – 04:45pm**      **Timothy Zwiernik**      (Sandia National Lab)  
*"Site-Specific Photochemistry out of Single Conformations of Cryo-cooled Ions: What can Gas Phase and Condensed Phase learn from one another?"*
- 04:45pm – 05:20pm**      **Veaceslav Coropceanu**      (University of Arizona)  
*"Manifestations of Electronic Hybridization on the Excited-state Properties of Donor-Acceptor Systems"*
- 05:20pm – 05:30pm**      **Closing Remarks**      Sergei Tretiak (LANL)