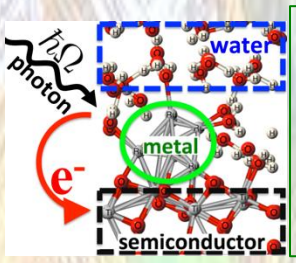
Computational Photocatalysis: Photophysics & Photochemistry at Interfaces. Machine Learning Bridges Theory and Experiment

Honolulu, Hawaii, December 16-17, 2025

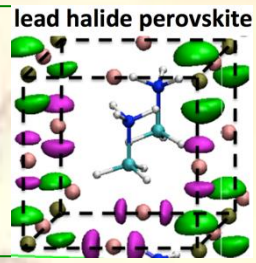
CTH005

- The symposium presents recent experimental, computational, and machine learning synergistic advances addressing the issue of charge transfer at the interfaces of nanomaterials for photovoltaic and photo-electrochemical applications.
- Symposium focuses at understanding the photoinduced processes of light absorption, formation and breaking of charge transfer excitations, hot carrier relaxation, and reaction dynamics at catalytic sites – affected by lattice vibrations and solvent polarization dynamics. These processes are monitored by femtosecond spectral methods and modeled using nonadibatic excited state dynamics.
- The efficiency of photo-catalytic and photovoltaic solar energy conversion is improved by active exploration of composition and morphology of nano-materials. Change of composition, quantum confinement, size, shape, surface functionalization, magnetic doping, and meso-scale structural arrangement provide versatile tuning of timescales of available basic mechanisms and properties of materials.



Focus

- Photo-induced dynamics in semiconductor nanostructures: confinement vs. doping
- Supported metal clusters for photocatalytic applications
- Photo-induced processes in functionalized metalooxide semiconductor surfaces
- New materials: Lead halide perovskites for photovoltaic applications



International Organizing Committee

Tsukasa Torimoto*, Nagoya University, Japan
Chuanyi Wang, Shaanxi Univ. Tech., China
Shuping Huang, Fuzhou U., China
Artur Izmaylov, U. Toronto, Canada
Koichi Yamashita, Yokohama City U., Japan
Masaru Kuno, Notre Dame, USA

Local organizers:

Dmitri Kilin, NDSU, USA
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Svetlana Kilina, NDSU, USA
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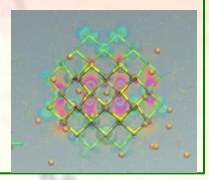
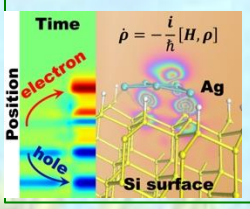
Advisory Committee: David Micha, University of Florida, USA

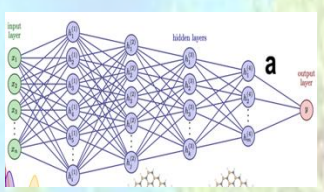


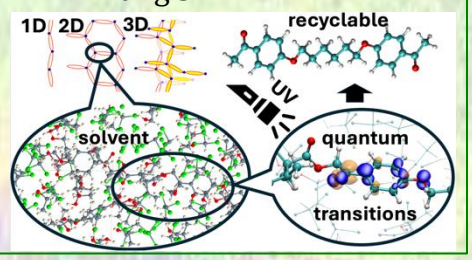
Tentative Invited Speakers

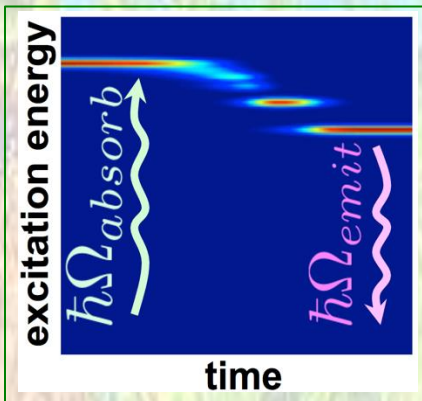
Victor Klimov*
Sharon Hammes-Schiffer*
Amanda Barnard
Teresa Head-Gordon
Nam-Gyu Pak
Peter Gill*
Sergei Tretiak*
Stephania Castelletto
Jadranka Travas-Sejdic
Koichi Yamashita
Ryoji Asahi
Ulrike Diebold
Sivaguru Jayaraman*
Giulia Galli*
Christine Aikens
Oleg Prezhdo*
Kazunari Domen*
Chuanyi Wang
Michael Graetzel
YuHuang Wang*
Michel Dupuis*
Anna Krylov*
Prashant Kamat*
Tsukasa Torimoto*
Margaret Reid
Anabella Selloni
Run Long*
Kwang S. Kim

*confirmed speakers









Abstract Submission Details

Submit at https://pacifichem2025.abstractcentral.com/submission

Division Topic Area: Computational and Theoretical (**CTH**) ,

Symposium Title: Computational Photocatalysis:
Photo-Physics & Photo-Chemistry at Interfaces.
Machine Learning Bridges Theory and Experiment

Symposium ID: **#CTH005** **Deadline: April 2, 2025**

Speakers are encouraged to accompany the talks by posters presented by a students.
Travel stipends to students may become available.