

Wednesday

## **ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry (2021): Symposium Honoring Kenneth D. Karlin:**

09:00am - 11:55am USA / Canada - Pacific - April 14, 2021

**Prof. Reza A. Ghiladi, PhD, Organizer, Presider** | **Eunsuk Kim, Organizer, Presider** | **Heather Lucas, Organizer**

### **Introductory Remarks**

09:00am - 09:05am USA / Canada - Pacific - April 14, 2021

Track: [INOR] Division of Inorganic Chemistry

Wednesday

### **Shining light on Karlin complexes**

09:05am - 09:30am USA / Canada - Pacific - April 14, 2021

**Gerald Meyer, Presenter**

### **Metal-oxo and metal-hydroxo (Fe, Mn) corrole model complexes: Insights regarding H-atom abstraction and radical rebound processes**

09:30am - 09:55am USA / Canada - Pacific - April 14, 2021

**David Goldberg, Presenter** | **Jan Paulo Zaragoza** | **Daniel Cummins** | **Jireh Joy Sacramento** | **Geoff Farley** | **Jithin Thomas**

### **Making a mouse roar like a lion: Turning a sluggish Fe(III)-OOH intermediate into a potent oxidant for cleaving strong C-H bonds**

09:55am - 10:20am USA / Canada - Pacific - April 14, 2021

**Shuangning Xu** | **Subhasree Kal** | **Waqas Rasheed** | **Apparao Darksharapu** | **Lawrence Que, Presenter**

Wednesday

### **Intermission**

10:20am - 10:35am USA / Canada - Pacific - April 14, 2021

Track: [INOR] Division of Inorganic Chemistry

Wednesday

### **Interpeptidic Cu(II) exchange – measuring exchange between model complexes and cull-amyloid-beta complexes using tryptophan fluorescence quenching**

10:35am - 11:00am USA / Canada - Pacific - April 14, 2021

**Debbie Crans, Presenter** | **Cheryle Beuning** | **Christelle Hureau**

### **Oxygen evolution from a transient thiolate-ligated Fe-superoxo intermediate**

11:00am - 11:25am USA / Canada - Pacific - April 14, 2021

**Professor Julie Kovacs, Presenter**

### **Activating metal sites for biological electron transfer**

11:25am - 11:50am USA / Canada - Pacific - April 14, 2021

**Edward Solomon, Presenter**

### **Concluding Remarks**

11:50am - 11:55am USA / Canada - Pacific - April 14, 2021

Wednesday

## **ACS Award in the Chemistry of Materials (2020): Symposium Honoring David Brian Mitzi:**

09:00am - 11:40am USA / Canada - Pacific - April 14, 2021

[David Ginger, Organizer, Presider](#) | [Bayrammurad Saparov, Organizer](#)

Wednesday

### [Tuning the electronic structure of layered hybrid organic-inorganic perovskites from first principles](#)

09:00am - 09:25am USA / Canada - Pacific - April 14, 2021

[Volker Blum, Presenter](#)

### [Hot exciton dynamics in two-dimensional organic-inorganic hybrid perovskites](#)

09:25am - 09:50am USA / Canada - Pacific - April 14, 2021

[Daniel Straus](#) | [Sebastian Hurtado Parra](#) | [Natasha Iotov](#) | [Qinghua Zhao](#) | [Michael Gau](#) | [Patrick Carroll](#) | [James Kikkawa](#) | [Cherie Kagan, Presenter](#)

### [Halide perovskite photophysics and device implications](#)

09:50am - 10:15am USA / Canada - Pacific - April 14, 2021

[Edward Sargent, Presenter](#)

### [Discussion](#)

10:15am - 10:25am USA / Canada - Pacific - April 14, 2021

### [High-efficiency light emission from all-inorganic copper halides](#)

10:25am - 10:50am USA / Canada - Pacific - April 14, 2021

[Bayrammurad Saparov, Presenter](#) | [Tielyr Creason](#) | [Mao-Hua Du](#)

### [Key role of the interface in the mechanochromic luminescence properties of hybrid perovskites](#)

10:50am - 11:15am USA / Canada - Pacific - April 14, 2021

[Nicolas Mercier, Presenter](#)

### [A theoretical perspective on the electronic and optical properties of layered halide perovskites: Symmetry analysis of quantum-well electronic structure and charge/energy transfer processes beyond the quantum-well picture](#)

11:15am - 11:40am USA / Canada - Pacific - April 14, 2021

[claudio quarti, Presenter](#) | [Mikael Kepenekian](#) | [Laurent Pedesseau](#) | [boubacar traoré](#) | [ferdinand ledée](#) | [pierre audebert](#) | [Emmanuelle Deleporte](#) | [Nicolas Mercier](#) | [Jacky Even](#) | [Claudine Katan](#)

Wednesday

### [Chemistry of Materials: Synthesis and Properties:](#)

09:00am - 11:20am USA / Canada - Pacific - April 14, 2021

[Claus Lugmair, Organizer](#) | [Alison Altman, Presider](#) | [Ebube Oyeka, Presider](#)

### [Soft processing toward layered and 2D materials: Expanding the palette](#)

09:00am - 09:20am USA / Canada - Pacific - April 14, 2021

[Dr David J. Lewis, Presenter](#)

### [Computationally directed discovery of MoBi2](#)

09:20am - 09:40am USA / Canada - Pacific - April 14, 2021

[Alison Altman, Presenter](#) | [Alexandra Tamerius](#) | [Nathan Koocher](#) | [Yue Meng](#) | [Chris Pickard](#) | [James Walsh](#) | [James Rondinelli](#) | [Steven Jacobsen](#) | [Danna Freedman](#)

### [Exploiting new chemical approaches to design magnetic skyrmions](#)

09:40am - 10:00am USA / Canada - Pacific - April 14, 2021

[Ebube Oyeka, Presenter](#) | [Michal Winiarski](#) | [Artur Blachowski](#) | [Keith Taddei](#) | [Allen Scheie](#) | [Thao Tran](#)

**[Bend or break, that is the question: Structure-property relationships in mechanically flexible co-crystals of N-\(5-halopyridin-2-yl\)alkylamides with aromatic carboxylic acids co-formers](#)**

10:00am - 10:20am USA / Canada - Pacific - April 14, 2021

[Amila Abeysekera, Presenter](#) | [Christer Aakeroy](#) | [Boris Averkiev](#) | [Abhijeet Sinha](#)

**[Toward durable multimetal oxyhalide intergrowths for solar water splitting](#)**

10:20am - 10:40am USA / Canada - Pacific - April 14, 2021

[Kaustav Chatterjee, Presenter](#) | [Roberto dos Reis](#) | [Jaye Harada](#) | [Jette Mathiesen](#) | [Sandra Bueno](#) | [Kirsten Jensen](#) | [James Rondinelli](#) | [Vinayak David](#) | [Sara Skrabalak](#)

**[Low-dimensional single-cation formamidinium lead halide perovskites \(FAM+2PbmBr3m+2\): From synthesis to rewritable phase-change memory film](#)**

10:40am - 11:00am USA / Canada - Pacific - April 14, 2021

[Duong Nguyen Minh, Presenter](#) | [Youngjong Kang](#)

**[Dihalomethane achievable nondestructive and controllable anion exchange for halide perovskite films](#)**

11:00am - 11:20am USA / Canada - Pacific - April 14, 2021

[Dr. Yu Chen, Presenter](#) | [Haotian Jiang](#) | [Haizheng Zhong](#)

Wednesday

**[Coordination Chemistry: Characterization and Applications:](#)**

09:00am - 12:00pm USA / Canada - Pacific - April 14, 2021

[Anna Larsen, Organizer](#) | [Dr. Mohammadreza Momenitaheri, Presider](#)

**[Coupling of diruthenium nitrides releases nitrogen gas](#)**

09:00am - 09:20am USA / Canada - Pacific - April 14, 2021

[Sungho Park, Presenter](#) | [Amanda Corcos](#) | [Alexander Jambor](#) | [Tzuhsiung Yang](#) | [John Berry](#)

**[Synthesis, structure and reactivity of three Ni\(N<sub>2</sub>S<sub>2</sub>\) redox states](#)**

09:20am - 09:40am USA / Canada - Pacific - April 14, 2021

[Yahya Albkuri, Presenter](#) | [Andrea Mulas](#) | [Jeffrey S. Ovens](#) | [Stephan Stephan Steinmann](#) | [Christophe Bucher](#) | [R Baker](#)

**[Modular design of multifunctionality in TCNQ-based Fe\(II\) spin crossover complexes](#)**

09:40am - 10:00am USA / Canada - Pacific - April 14, 2021

[Okten Ungor, Presenter](#) | [Eun Sang Choi](#) | [Michael Shatruk](#)

**[Palladium deposited on a layered covalent-organic framework: The role of local defects in the catalytic activity for Suzuki–Miyaura cross-coupling reactions](#)**

10:00am - 10:20am USA / Canada - Pacific - April 14, 2021

[Ignacio Romero-Muñiz](#) | [Andreas Mavrandonakis](#) | [Pablo Albacete](#) | [Alicia Vega](#) | [Valérie Briois](#) | [Felix Zamora](#) | [Dr. Ana Eva P. Platero Prats, Presenter](#)

**[Modulating optical properties of BODIPY aggregates encapsulated in coordination cages](#)**

10:20am - 10:40am USA / Canada - Pacific - April 14, 2021

[Dr. Mohammadreza Momenitaheri, Presenter](#) | [David Dell'Angelo](#) | [Farnaz Shakib](#)

### [Temperature-dependent metal complexes synthesis of vitamin K3 analog phthiocol \(2-hydroxy-3-methylnaphthalene-1,4-dione\), evaluation of the anticancer activity](#)

10:40am - 11:00am USA / Canada - Pacific - April 14, 2021

[Dr. Surekha K. Satpute, Assistant Professor, Presenter](#) | [Dr. sunita A. Salunke, Professor, Presenter](#) | [Shital Harihar](#) | [Nishigandha Mone](#)

### [Improved photoreactivity through the expansion of unfavorable Ru-N bite angles on \[Ru\(dppz\)\(tpy\)\]<sup>2+</sup> type complexes](#)

11:00am - 11:20am USA / Canada - Pacific - April 14, 2021

[Austin Lanquist, Presenter](#) | [Eric Piechota](#) | [Claudia Turro](#)

### [Atomic-resolution imaging of coordination compounds on graphene](#)

11:20am - 11:40am USA / Canada - Pacific - April 14, 2021

[Blanka E. Janicek, Presenter](#) | [Priti Kharel](#) | [Sang hyun Bae](#) | [Amanda Loutris](#) | [Pinshane Huang](#)

### [Controlling the conversion of magnesium aminodiborates to superconducting MgB<sub>2</sub>](#)

11:40am - 12:00pm USA / Canada - Pacific - April 14, 2021

[Chris Caroff, Presenter](#) | [Justin Mallek](#) | [Brian Bellott](#) | [Gregory Girolami](#)

Wednesday

## [Organometallic Chemistry: Synthesis and Characterization - Early Transition Metals:](#)

09:00am - 10:40am USA / Canada - Pacific - April 14, 2021

[Nora Radu, Organizer](#) | [Rebecca Siegelman, Presider](#)

### [Successful synthesis of the first all-C-deprotonated cyclobutadiene?](#)

09:00am - 09:20am USA / Canada - Pacific - April 14, 2021

[Fabian Reiss, Presenter](#) | [Melanie Reiss](#) | [Jonas Bresien](#) | [Anke Spannberg](#) | [Haijun Jiao](#) | [Wolfgang Baumann](#) | [Perdita Arndt](#) | [Torsten Beweries](#)

### [Cobalt mediated regioselectivity in Pauson-Khand reaction a possible Co-N participation and oxidative 6Pi-electrocyclization / aromatization reactions](#)

09:20am - 09:40am USA / Canada - Pacific - April 14, 2021

[Nasiru Yahaya, Presenter](#)

### [Low valent Ti complexes stabilized by arene-linked bisphenoxide ligands](#)

09:40am - 10:00am USA / Canada - Pacific - April 14, 2021

[Steven Butler, Presenter](#) | [Ian Tonks](#)

### [Activation of dinitrogen by a titanium complex with an amino triphenolate ligand lead by geometry shift](#)

10:00am - 10:20am USA / Canada - Pacific - April 14, 2021

[Dae Young Bae, Presenter](#) | [Gunhee Lee](#) | [Eunsung Lee](#)

### [Quantum yield studies of C-H bond activation by a Mo\(VI\) dioxo complex](#)

10:20am - 10:40am USA / Canada - Pacific - April 14, 2021

[Siddhiaratchi Dinushini Siddhiaratchi, Presenter](#) | [Matthew Chambers](#)

Wednesday

### [How Can the DIC be Better for You?](#)

12:00pm - 01:00pm USA / Canada - Pacific - April 14, 2021 | Room: Virtual Room

Wednesday

### [ACS Award in the Chemistry of Materials \(2020\): Symposium Honoring David Brian Mitzi:](#)

01:00pm - 03:15pm USA / Canada - Pacific - April 14, 2021

[David Ginger, Organizer, Presider](#) | [Bayrammurad Saparov, Organizer, Presider](#)

### [From lead halide perovskites to lead-free metal halide perovskites](#)

01:00pm - 01:25pm USA / Canada - Pacific - April 14, 2021

[Yanfa Yan, Presenter](#)

### [Increasing the complexity of halide perovskites](#)

01:25pm - 01:50pm USA / Canada - Pacific - April 14, 2021

[Kurt Lindquist](#) | [Michael Boles](#) | [Daiki Umeyama](#) | [Bridget Connor](#) | [Adam Slavney](#) | [Linn Leppert](#) | [Hemamala Karunadasa, Presenter](#)

### [Lone pairs in the halide perovskites, hidden or otherwise](#)

01:50pm - 02:15pm USA / Canada - Pacific - April 14, 2021

[Professor Ram Seshadri, Presenter](#)

### [Discussion](#)

02:15pm - 02:25pm USA / Canada - Pacific - April 14, 2021

### [Carrier-resolved photo hall effect and its application in high performance perovskite solar absorber](#)

02:25pm - 02:50pm USA / Canada - Pacific - April 14, 2021

[Oki Gunawan, Presenter](#) | [Byungha Shin](#) | [David Mitzi](#)

### [Ion transport in halide perovskites: Dimensionality, ions, and electronic carriers](#)

02:50pm - 03:15pm USA / Canada - Pacific - April 14, 2021

[David Ginger, Presenter](#)

Wednesday

### [Chemistry of Materials: Synthesis and Properties:](#)

01:00pm - 03:00pm USA / Canada - Pacific - April 14, 2021

[Claus Lugmair, Organizer](#) | [Kailash Arole, Presider](#)

### [Exploring the properties of Boron difluoride hydrazones as small molecules and polymers](#)

01:00pm - 01:20pm USA / Canada - Pacific - April 14, 2021

[Daniela Cappello, Presenter](#) | [Ryan Maar](#) | [Alexander Watson](#) | [Denis Therien](#) | [Francois Lagugne-Labarthet](#) | [Viktor Staroverov](#) | [Joe Gilroy](#)

### [Amine-substituted near-infrared boron difluoride formazanate dyes](#)

01:20pm - 01:40pm USA / Canada - Pacific - April 14, 2021

[Francis Buguis, Presenter](#) | [Ryan Maar](#) | [Viktor Staroverov](#) | [Joe Gilroy](#)

### [Intercalation chemistry of mixed anionic materials](#)

01:40pm - 02:00pm USA / Canada - Pacific - April 14, 2021

[Andrew Smith, Presenter](#) | [Brian Leonard](#)

### [Synthesis and speciation of Co<sup>2+</sup> dopants in \[Cd<sub>10</sub>S<sub>4</sub>\(SPh\)<sub>16</sub>\]<sub>4</sub>- clusters from a self-assembly route](#)

02:00pm - 02:20pm USA / Canada - Pacific - April 14, 2021

[Jillian Denhardt, Presenter](#) | [Kevin Kittilstved](#)

### [Impact of ethyl cellulose on the porosity and capacitance of CuGaO<sub>2</sub> mesoporous nanocrystalline thin films](#)

02:20pm - 02:40pm USA / Canada - Pacific - April 14, 2021

[Humaira Yeasmin, Presenter](#) | [Alexandria Combs Bredar](#) | [Byron Farnum](#)

### [Synthesis of water-dispersible Ti<sub>3</sub>C<sub>2</sub>T<sub>z</sub> MXene nanosheets by molten salt etching](#)

02:40pm - 03:00pm USA / Canada - Pacific - April 14, 2021

[Kailash Arole, Presenter](#) | [Jackson Bilvin](#) | [Sanjit Saha](#) | [Micah Green](#) | [Miladin Radovic](#) | [Jodie Lutkenhaus](#)

Wednesday

### [Coordination Chemistry: Synthesis and Characterization:](#)

01:00pm - 04:00pm USA / Canada - Pacific - April 14, 2021

[Anna Larsen, Organizer](#) | [Brian Lindley, Presider](#) | [John Gary, Presider](#)

### [Cyclic diborylamide complexes of lithium and first-row transition metals](#)

01:00pm - 01:20pm USA / Canada - Pacific - April 14, 2021

[Brian Lindley, Presenter](#)

### [Pyridoxal based chemosensors for zinc ions sensing in aqueous media: Synthesis, crystallography, and optical properties](#)

01:20pm - 01:40pm USA / Canada - Pacific - April 14, 2021

[Anwar Hussain, Presenter](#) | [Dawson C. Cork](#) | [Luke Lewandowski](#) | [Kadarkaraisamy Mariappan](#) | [Andrew G. Sykes](#)

### [Exploring the electronic structure of novel Ru<sup>2+</sup> paddlewheel complexes](#)

01:40pm - 02:00pm USA / Canada - Pacific - April 14, 2021

[Michael D. Roy, Presenter](#) | [John Berry](#)

### [Pincer-ligated manganese dicarbonyl complexes featuring an N-heterocyclic phosphonium/phosphido moiety](#)

02:00pm - 02:20pm USA / Canada - Pacific - April 14, 2021

[Leah Oliemuller, Presenter](#) | [Christine Thomas](#)

### [Computational analysis of N<sub>2</sub>O binding to metal complexes](#)

02:20pm - 02:40pm USA / Canada - Pacific - April 14, 2021

[Kylie Fields](#) | [Brian Barngrover](#) | [John Gary, Presenter](#)

### [Bimetallic iron–tin catalyst for N<sub>2</sub> to NH<sub>3</sub> and a silyldiazenido model intermediate](#)

02:40pm - 03:00pm USA / Canada - Pacific - April 14, 2021

[Michael Dorantes, Presenter](#) | [James Moore](#) | [Eckhard Bill](#) | [Bernd Mienert](#) | [Connie Lu](#)

**Synthesis, characterization, crystal structures of novel di-(2-picoyl) amine appended rigid phenyl based and non-rigid 1,4-benzodioxan based ring systems and their Pt (II) complexes towards potential biological applications**

03:00pm - 03:20pm USA / Canada - Pacific - April 14, 2021

[Dinithi Kaluthanthiri, Presenter](#) | [Frank Fronczek](#) | [Laksiri Weerasinghe](#) | [Theshini Perera](#)

**Sulfur-centered reactions of a zinc tetrasulfanido complex: Redox and sulfur atom transfer**

03:20pm - 03:40pm USA / Canada - Pacific - April 14, 2021

[Moises Ballesteros, Presenter](#) | [Emily Tsui](#)

**Review study on Cu(II) metal complexes of Pyridyl based Schiff bases and their biological importance**

03:40pm - 04:00pm USA / Canada - Pacific - April 14, 2021

[Dr. Suman Malik, Head, Department of Chemistry, Presenter](#)

Wednesday

**Environmental and Energy-related Inorganic Chemistry:**

01:00pm - 04:00pm USA / Canada - Pacific - April 14, 2021

[Dr Stephen A. Koch, Organizer](#) | [Andrew Maverick, Presider](#) | [Matthew Chambers, Presider](#)

**Computational screening of stable, highly efficient and non-toxic inorganic halide double perovskites for photovoltaic applications**

01:00pm - 01:20pm USA / Canada - Pacific - April 14, 2021

[Moses Bokinala, Presenter](#) | [Showkat Mir](#) | [Jayant Singh](#)

**o-Sulfonamidophenol ligands for f-element sensing and separation from alkaline high-level waste.**

01:20pm - 01:40pm USA / Canada - Pacific - April 14, 2021

[Oluwaseun W. Adedoyin, Presenter](#) | [Alexander N. Morozov](#) | [Alexander Mebel](#) | [Konstantinos Kavallieratos](#)

**Complexation, extraction, and sensing of Hg(II) by sulfonamide ligands derived from o-phenylenediamine**

01:40pm - 02:00pm USA / Canada - Pacific - April 14, 2021

[Adenike Fasiku, Presenter](#) | [Indranil Chakraborty](#) | [René Panzer](#) | [Raphael Raptis](#) | [Konstantinos Kavallieratos](#)

**Using light to control light hydrocarbon functionalization with Group VI dioxo complexes**

02:00pm - 02:20pm USA / Canada - Pacific - April 14, 2021

[Matthew Chambers, Presenter](#)

**Vibrational relaxation dynamics in layered 2D perovskites**

02:20pm - 02:40pm USA / Canada - Pacific - April 14, 2021

[Li Na Quan, Presenter](#)

**Electrochemical reduction of chromate in buffered acid solutions for water purification**

02:40pm - 03:00pm USA / Canada - Pacific - April 14, 2021

[Callie Stern, Presenter](#) | [Darius Hayes](#) | [Lebo Kgoadi](#) | [Noemie Elgrishi](#)

### [Are Cu\(II\) oxalate complexes formed by reduction of CO<sub>2</sub> or oxidation of ascorbate?](#)

03:00pm - 03:20pm USA / Canada - Pacific - April 14, 2021

[Fatemeh Khamespanah](#) | [Maximilian Marx](#) | [David Crochet](#) | [Uttam Pokharel](#) | [Frank Fronczek](#) | [Andrew Maverick, Presenter](#) | [Matthias Beller](#)

### [Exploring the oxidative quenching pathways of iridium \(III\) photocatalysts with high-throughput experimentation: A path to carbon-neutral solar hydrogen](#)

03:20pm - 03:40pm USA / Canada - Pacific - April 14, 2021

[Velabo Mdluli, Presenter](#) | [Stephen DiLuzio](#) | [Stefan Bernhard](#)

### [Trends for first row transition metal complexes for binding carbon dioxide](#)

03:40pm - 04:00pm USA / Canada - Pacific - April 14, 2021

[Emily Landgreen, Presenter](#) | [Hayley Petras](#) | [Samantha Country](#) | [Collin Sindt](#) | [James Shepherd](#)

Wednesday

### [Inorganic Catalysts:](#)

01:00pm - 04:00pm USA / Canada - Pacific - April 14, 2021

[Dr Stephen A. Koch, Organizer](#) | [Dr. Lei Wang, Presider](#) | [Bess Vlasisavljevich, Presider](#)

### [Is \$\pi\$ -loading real: And, if so, could it be used in catalyst design?](#)

01:00pm - 01:20pm USA / Canada - Pacific - April 14, 2021

[Catherine Moulder, Presenter](#) | [Thomas Cundari](#)

### [Olefin polymerization by zirconium boratabenzene catalysts](#)

01:20pm - 01:40pm USA / Canada - Pacific - April 14, 2021

[Carly Carter, Presenter](#) | [Thomas Cundari](#) | [George Rodriguez](#)

### [Vanadium pnictide and chalcogenide complexes supported by the scorpionate TptBu<sub>2</sub>Me ligand](#)

01:40pm - 02:00pm USA / Canada - Pacific - April 14, 2021

[Mehrafshan Jafari, Presenter](#) | [Dominik Fehn](#) | [Cristina Prieto](#) | [Prajay Patel](#) | [Cong Liu](#) | [Anders Reinholdt](#) | [Arthur Kropf](#) | [David Kaphan](#) | [Michael Gau](#) | [Patrick Carroll](#) | [Jurek Krzystek](#) | [Andrew Ozarowski](#) | [Joshua Telser](#) | [Massimiliano Delferro](#) | [Karsten Meyer](#) | [Daniel Mindiola](#)

### [Computational insights into the nucleation and electrochemistry of polyoxovanadate-alkoxide clusters](#)

02:00pm - 02:20pm USA / Canada - Pacific - April 14, 2021

[Pere Miro, Presenter](#)

### [DFT-based mechanistic insights of an indium-catalyzed green reaction : Key learnings from orbital analysis](#)

02:20pm - 02:40pm USA / Canada - Pacific - April 14, 2021

[PARVEEN Rawal, Presenter](#)

### [Catalytic dehydrogenation of formamides to isocyanates with PNP-Ru pincer complexes](#)

02:40pm - 03:00pm USA / Canada - Pacific - April 14, 2021



[Abebu Kassie, Presenter](#) | [Matthew Remy](#) | [Sukrit Mukhopadhyay](#) | [Melanie Sanford](#)

### [High redox potential chromophores for visible light-driven water oxidation at low pH](#)

03:00pm - 03:20pm USA / Canada - Pacific - April 14, 2021

[Dr. Lei Wang, Presenter](#) | [Javier Concepcion](#)

### [Mechanistic cooperativity for water reduction with homobimetallic cobalt and nickel catalysts](#)

03:20pm - 03:40pm USA / Canada - Pacific - April 14, 2021

[Fredricka Morgan, Presenter](#) | [Claudio Verani](#)

### [Electronic structure and oxidation state in two copper catalysts](#)

03:40pm - 04:00pm USA / Canada - Pacific - April 14, 2021

[Bess Vlasisavljevich, Presenter](#)

Wednesday

### [Main Group Chemistry:](#)

01:00pm - 03:30pm USA / Canada - Pacific - April 14, 2021

[Todd Hudnall, Organizer, Presider](#)

### [Molecular cubism: Design of higher valency in covalent organic frameworks](#)

01:00pm - 01:20pm USA / Canada - Pacific - April 14, 2021

[Cornelius Gropp, Presenter](#) | [Tianqiong Ma](#) | [Nikita Hanikel](#) | [Omar Yaghi](#)

### [\[XeF<sub>5</sub>\]<sup>+</sup> and \[Xe<sub>2</sub>F<sub>11</sub>\]<sup>+</sup> Salts of the group 6 oxyfluoro-anions \[Cr<sub>2</sub>O<sub>2</sub>F<sub>8</sub>\]<sup>2-</sup>, \[CrOF<sub>5</sub>\]<sup>-</sup>, \[MOF<sub>5</sub>\]<sup>-</sup> \(M = Mo, W\), and \[M<sub>2</sub>O<sub>2</sub>F<sub>9</sub>\]<sup>-</sup>](#)

01:20pm - 01:40pm USA / Canada - Pacific - April 14, 2021

[Mark R. Bortolus, Presenter](#) | [Helene Mercier](#) | [Gary Schrobilgen](#)

### [Frustrated Lewis Pair ligation for low-temperature semiconductor element and polymer deposition](#)

01:40pm - 02:00pm USA / Canada - Pacific - April 14, 2021

[Alvaro Omana, Presenter](#) | [Rachel Green](#) | [Ryo Kobayashi](#) | [Yingjie He](#) | [Evan Antoniuk](#) | [Michael Ferguson](#) | [Yuqiao Zhou](#) | [Jonathan Veinot](#) | [Takeaki Iwamoto](#) | [Alexander Brown](#) | [Eric Rivard](#)

### [Synthesis and characterization of transition metal malondiiminates](#)

02:00pm - 02:20pm USA / Canada - Pacific - April 14, 2021

[Claire Schmit, Presenter](#) | [Gregory Girolami](#)

### [Intermission](#)

02:20pm - 02:30pm USA / Canada - Pacific - April 14, 2021

### [Revealing unusual reaction pathways via halogen bonding](#)

02:30pm - 02:50pm USA / Canada - Pacific - April 14, 2021

[Andrew Peloquin, Presenter](#) | [Colin McMillen](#) | [Scott Iacono](#) | [William Pennington](#)

### [Beyond BOPs: Exploring functional materials derived from 1,3-benzoxaphospholes](#)

02:50pm - 03:10pm USA / Canada - Pacific - April 14, 2021

[Zakary Ekstrom, Presenter](#) | [John Protasiewicz](#)

**Highly accurate benchmarking and characterization of donor-acceptor interactions in molecular systems containing dative bonds**

03:10pm - 03:30pm USA / Canada - Pacific - April 14, 2021

**Brett Smith, Presenter**

**Bioinorganic Social Hour**

04:00pm - 05:00pm USA / Canada - Pacific - April 14, 2021

Wednesday

**ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry (2021): Symposium Honoring Kenneth D. Karlin:**

05:00pm - 07:55pm USA / Canada - Pacific - April 14, 2021

**Prof. Reza A. Ghiladi, PhD, Organizer** | **Eunsuk Kim, Organizer** | **Heather Lucas, Organizer** | **Prof. Yunho Lee, Presider** | **Jun Wang, Presider**

**Introductory Remarks**

05:00pm - 05:05pm USA / Canada - Pacific - April 14, 2021

**Biomimetic metal-oxygen intermediates in dioxygen activation chemistry**

05:05pm - 05:30pm USA / Canada - Pacific - April 14, 2021

**Wonwoo Nam, Presenter**

**Bioinorganic strategies to study multiple facets in Alzheimer's disease**

05:30pm - 05:55pm USA / Canada - Pacific - April 14, 2021

**Mi Hee Lim, Presenter**

**Bioinspired organometallic catalysis of 1st-row transition metals**

05:55pm - 06:20pm USA / Canada - Pacific - April 14, 2021

**Prof. Yunho Lee, Presenter**

**Intermission**

06:20pm - 06:35pm USA / Canada - Pacific - April 14, 2021

**Catalytic alkane hydroxylation by transition-metal/acylperoxide systems**

06:35pm - 07:00pm USA / Canada - Pacific - April 14, 2021

**Shinobu Itoh, Presenter**

**Structures and characterization of manganese(III) peroxido complexes ligated by highly hindered N3 type ligands**

07:00pm - 07:25pm USA / Canada - Pacific - April 14, 2021

**Kiyoshi Fujisawa, Presenter** | **Riko Ikarugi** | **Syuhei Sakuma**

**NO : a potential biomarker for autism spectrum disorder children and their parents**

07:25pm - 07:50pm USA / Canada - Pacific - April 14, 2021

**Wang Jun, Presenter** | **Lulu Yao** | **Lu Bai** | **Ai Shi** | **Gong Miaozi** | **Shenghan Lai**

**Concluding Remarks**

07:50pm - 07:55pm USA / Canada - Pacific - April 14, 2021

Wednesday

### Chemistry of Materials: Materials for Energy and Catalytic Applications:

05:00pm - 07:40pm USA / Canada - Pacific - April 14, 2021

[Claus Lugmair, Organizer](#) | [Prof. Audrey Moores, Presider](#) | [Blaine Fiss, Presider](#)

### Withdrawn

05:00pm - 05:20pm USA / Canada - Pacific - April 14, 2021

### Host-guest composite materials: Electro-catalytic water splitting and aerial carbon dioxide capture

05:20pm - 05:40pm USA / Canada - Pacific - April 14, 2021

[Samar Das, Presenter](#)

### Using TD-DFT to characterize active sites on copper-exchanged zeolites

05:40pm - 06:00pm USA / Canada - Pacific - April 14, 2021

[Kevin Curtis, Presenter](#) | [Dipak Panthi](#) | [Samuel Odoh](#)

### The effect of formamide on the synthesis of metal hydroxide electrocatalysts

06:00pm - 06:20pm USA / Canada - Pacific - April 14, 2021

[Elif Pinar Alsac, Presenter](#) | [Rodney Smith](#)

### Carbon dots for photocatalytic H<sub>2</sub> production in aqueous media with molecular Co catalysts

06:20pm - 06:40pm USA / Canada - Pacific - April 14, 2021

[Dr. Kalliopi Ladomenou, Presenter](#) | [Georgios Landrou](#) | [Georgios Charalambidis](#) | [Emmanouil Nikoloudakis](#) | [Athanasios Coutsolelos](#)

### Room temperature, mechanochemical synthesis of ultrasmall nickel phosphide hydrogen evolution catalysts

06:40pm - 07:00pm USA / Canada - Pacific - April 14, 2021

[Blaine Fiss, Presenter](#) | [Nhu-Nang Vu](#) | [Georgia Douglas](#) | [Trong-On Do](#) | [Tomislav Friscic](#) | [Prof. Audrey Moores](#)

### Investigation of energetic solid-state metathesis reactions for the formation of iron, cobalt and nickel borides and their electrocatalytic activities

07:00pm - 07:20pm USA / Canada - Pacific - April 14, 2021

[Janaka Abeysinghe, Presenter](#) | [Edward Gillan](#)

### Plasmonic catalysis take on H<sub>2</sub> and O<sub>2</sub> activation

07:20pm - 07:40pm USA / Canada - Pacific - April 14, 2021

[Luis de La Garza](#) | [Alexandra Gellé](#) | [Michael Landry](#) | [Raynald Gauvin](#) | [Zacharias Amara](#) | [Prof. Audrey Moores, Presenter](#) | [Christopher Barrett](#)

Wednesday

### Solid-State Inorganic Chemistry:

05:00pm - 08:00pm USA / Canada - Pacific - April 14, 2021

[Viktor V. Poltavets, Ph.D., Organizer, Presider](#)

### Synthesis, structure, and physicochemical characterization of novel quaternary lanthanide-chalcogenides with noncentrosymmetric structure and potential in IR-NLO applications

05:00pm - 05:20pm USA / Canada - Pacific - April 14, 2021

[Andrew Craig, Presenter](#) | [Stanislav Stoyko](#) | [Jennifer Aitken](#)

### [Silicate-analogous borosulfates featuring promising luminescence and frequency-doubling \(SHG\) properties based on a rich crystal chemistry](#)

05:20pm - 05:40pm USA / Canada - Pacific - April 14, 2021

[Philip Netzsch](#) | [Matthias Hämmer](#) | [Peter Gross](#) | [Henning A. Hoppe, Presenter](#)

### [Spectroscopic Examination of the Tunable Valency of Mn Dopants in Strontium Titanate-based Powders](#)

05:40pm - 06:00pm USA / Canada - Pacific - April 14, 2021

[Haneen Mansoor, Presenter](#) | [Keith Lehuta](#) | [Kevin Kittilstved](#)

### [Analysis of solid-state reaction mechanisms with two-dimensional FTIR correlation spectroscopy](#)

06:00pm - 06:20pm USA / Canada - Pacific - April 14, 2021

[Rodney Smith, Presenter](#)

### [Intermission](#)

06:20pm - 06:40pm USA / Canada - Pacific - April 14, 2021

### [Exploring novel binary copper oxides using density functional theory and evolutionary algorithms](#)

06:40pm - 07:00pm USA / Canada - Pacific - April 14, 2021

[Sankari Sampath, Presenter](#) | [Kamil Tokar](#) | [Mariana Derzsi](#)

### [Discovering and characterizing new functional ferroelectric and antiferroelectric materials using computers](#)

07:00pm - 07:20pm USA / Canada - Pacific - April 14, 2021

[Autumn Cook, Presenter](#) | [Aaliyah Khan](#) | [Joseph Bennett](#)

### [Synthesis of europium selenide nanocrystals and observations of conduction band-splitting](#)

07:20pm - 07:40pm USA / Canada - Pacific - April 14, 2021

[Dane Romar Asuigui, Presenter](#) | [Sarah Stoll](#) | [Michael de Siena](#) | [Rachel Fainblat](#) | [Derak James](#) | [Daniel R. Gamelin](#)

### [Development and validation of ReaxFF forcefield for solid-state ion conduction in Ag/S-based systems](#)

07:40pm - 08:00pm USA / Canada - Pacific - April 14, 2021

[Calvin Anderson, Presenter](#) | [John Rakovan](#) | [Mehdi Zanjani](#)

Wednesday

### [Organometallic Chemistry: Catalysis-Late Transition Metals:](#)

05:00pm - 07:40pm USA / Canada - Pacific - April 14, 2021

[Nora Radu, Organizer](#) | [Ryan Trovitch, Presider](#)

### [Dynamics of re-mediated ethylene C-H activation](#)

05:00pm - 05:20pm USA / Canada - Pacific - April 14, 2021

[Bo Yang, Presenter](#) | [Anna Schouten](#) | [Daniel Ess](#)

### [Copper\(II\) ketimides in sp<sup>3</sup> C-H functionalization](#)

05:20pm - 05:40pm USA / Canada - Pacific - April 14, 2021

[Isuri Jayasooriya, Presenter](#) | [Abolghasem Bakhoda](#) | [Rachel Palmer](#) | [Kristi Ng](#) | [Nour Kaschmoune](#) | [Jeffery Bertke](#) | [Timothy Warren](#)

### [Cobalt catalyzed \$\alpha\$ -alkylation and olefination of nitriles with primary alcohols](#)

05:40pm - 06:00pm USA / Canada - Pacific - April 14, 2021

[Keshav Paudel, Presenter](#) | [Keying Ding](#)

### [Catalytic azide-alkyne cycloaddition using multinuclear copper\(I\) pyrazolates](#)

06:00pm - 06:20pm USA / Canada - Pacific - April 14, 2021

[Monika Patterson, Presenter](#) | [Rasika Dias](#)

### [How does electron count influence base metal hydrosilylation activity?](#)

06:20pm - 06:40pm USA / Canada - Pacific - April 14, 2021

[Ryan Trovitch, Presenter](#)

### [First-row transition metal complexes for electrocatalytic oxidation of liquid fuels](#)

06:40pm - 07:00pm USA / Canada - Pacific - April 14, 2021

[Kate Waldie, Presenter](#)

### [Illuminating Nil cyclam's catalytic machinery: characterization of ligand-dependent small molecule activation with infrared spectroscopy and temperature-programmed ion chemistry](#)

07:00pm - 07:20pm USA / Canada - Pacific - April 14, 2021

[Dr. Sean C. Edington, Presenter](#) | [Evan Perez](#) | [David Charboneau](#) | [Fabian Menges](#) | [Nilay Hazari](#) | [Mark Johnson](#)

### [Exploration of cobalt catalysts for the electro-oxidation of liquid fuels](#)

07:20pm - 07:40pm USA / Canada - Pacific - April 14, 2021

[Andrew W. Cook, Presenter](#) | [Sriram Katipamula](#) | [Kate Waldie](#)

Wednesday

### [ACS Award for Encouraging Women into Careers in the Chemical Sciences: Symposium Honoring Katherine Franz :](#)

05:00pm - 08:00pm USA / Canada - Pacific - April 14, 2021

[Debbie Crans, Organizer](#) | [Louise Charkoudian, Presider](#) | [Annastassia Gallo, Presider](#)

### [Introductory Remarks](#)

05:00pm - 05:05pm USA / Canada - Pacific - April 14, 2021

### [Capturing transient interactions of proteins involved in natural product biosynthesis](#)

05:05pm - 05:24pm USA / Canada - Pacific - April 14, 2021

[Louise Charkoudian, Presenter](#)

### [Chaperoning Mischievous copper in extracellular spaces](#)

05:24pm - 05:43pm USA / Canada - Pacific - April 14, 2021

[Kathryn L. Haas, Ph.D., Presenter](#)

### [Changes to Candida albicans' metalloproteome as a result of azole drug stress](#)

05:43pm - 05:58pm USA / Canada - Pacific - April 14, 2021

[Catherine Denning, Presenter](#) | [Elizabeth Hunsaker](#) | [Larissa Lago](#) | [Blaine Roberts](#) | [Prof. Katherine J. Franz](#)

### [Microbial genome screening for siderophore biosynthetic pathways](#)

05:58pm - 06:17pm USA / Canada - Pacific - April 14, 2021

[Alison Butler, Presenter](#) | [Zachary Reitz](#)

### [Homeostasis and trafficking of titanium with cells, proteins, and small molecules](#)

06:17pm - 06:36pm USA / Canada - Pacific - April 14, 2021

[Ann Valentine, Presenter](#)

### [Anticancerous non-innocent vanadium Schiff base complexes](#)

06:36pm - 06:54pm USA / Canada - Pacific - April 14, 2021

[Debbie Crans, Presenter](#) | [Aviva Levina](#) | [Peter Lay](#)

### [A bioinorganic approach to photoresponsive materials: V and Fe coordination in polysaccharides](#)

06:54pm - 07:12pm USA / Canada - Pacific - April 14, 2021

[Alexis Ostrowski, Presenter](#) | [Carina Haddad](#) | [Kalani Edirisinghe](#)

### [Artificial iron proteins using biotin-streptavidin technology](#)

07:12pm - 07:27pm USA / Canada - Pacific - April 14, 2021

[Kelsey Miller, Presenter](#) | [Andrew Borovik](#)

### [Gold catalysts to cross-couple them all](#)

07:27pm - 07:42pm USA / Canada - Pacific - April 14, 2021

[Sophie Thomas, Presenter](#)

### [Alkali metal cation effects on intermediates and products of C-H bond oxidation chemistry effected by {Cun-O2} moieties](#)

07:42pm - 08:00pm USA / Canada - Pacific - April 14, 2021

[Sarah Brazeau](#) | [Emily Norwine](#) | [Nathaniel Hartmann](#) | [Prof. Linda H. Doerr, Presenter](#)