

Day 7 Programming

Tuesday

ACS National Awards Plenary Sessions:

09:00am - 12:00pm USA / Canada - Pacific - April 13, 2021

[Alison Butler, Organizer, Presider](#) | [Dr Stephen A. Koch, Organizer](#) | [Nora Radu, Organizer](#) | [Andy Borovik, Presider](#) | [Ana De Bettencourt Dias, Presider](#)

Tuesday

Ligand-copper and porphyrinate-iron coordination complexes with molecular oxygen and its reduced derivatives

09:00am - 09:45am USA / Canada - Pacific - April 13, 2021

[Kenneth Karlin, Presenter](#)

Infectiously inorganic: A metallocentric and mentoring-centric view of advancing bioinorganic chemistry at the host-pathogen interface

09:45am - 10:30am USA / Canada - Pacific - April 13, 2021

[Prof. Katherine J. Franz, Presenter](#)

Halide perovskites: Unprecedented opportunities (and some challenges) for semiconductor design and application

10:30am - 11:15am USA / Canada - Pacific - April 13, 2021

[David Mitzi, Presenter](#)

Catalysis with iron and cobalt: New applications and opportunities

11:15am - 12:00pm USA / Canada - Pacific - April 13, 2021

[Professor Paul J. Chirik, Presenter](#)

Tuesday

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

01:00pm - 04:00pm USA / Canada - Pacific - April 13, 2021

[Prof. Reza A. Ghiladi, PhD, Organizer, Presider](#) | [Eunsuk Kim, Organizer](#) | [Heather Lucas, Organizer, Presider](#)

Tuesday

Introductory Remarks

01:00pm - 01:05pm USA / Canada - Pacific - April 13, 2021

Tuesday

Mechanistic pathways in 3d-based catalysts for proton/water reduction

01:05pm - 01:30pm USA / Canada - Pacific - April 13, 2021

[Claudio Verani, Presenter](#)

Revisiting an old friend: Spectroscopic, structural, and electrochemical studies of ferricenium derivatives with weakly coordinating anions

01:30pm - 01:55pm USA / Canada - Pacific - April 13, 2021

[Shabnam Hematian, Presenter](#) | [Firoz Khan](#) | [Amy Waldbusser](#) | [Maria Carrasco](#) | [Hadi Pourhadi](#)

The Mechanism of Superoxide Reduction in Nickel Containing Superoxide Dismutase

01:55pm - 02:20pm USA / Canada - Pacific - April 13, 2021

[Jason Shearer, Presenter](#)

Tuesday

Intermission

02:20pm - 02:25pm USA / Canada - Pacific - April 13, 2021

Tuesday

Investigation of redox potential effects on the reactivity of primary copper(I)-dioxxygen adducts

02:25pm - 02:45pm USA / Canada - Pacific - April 13, 2021

[Austin Herzog, Presenter](#) | [Kenneth Karlin](#)

Characterization of a thioether-ligated cupric superoxide model complex with hydrogen atom abstraction reactivity

02:45pm - 03:05pm USA / Canada - Pacific - April 13, 2021

[Mayukh Bhadra, Presenter](#) | [Kenneth Karlin](#)

A mononuclear copper hydroxide core in three molecular oxidation states

03:05pm - 03:30pm USA / Canada - Pacific - April 13, 2021

[Isaac Garcia-Bosch, Presenter](#)

Controlling α -synuclein assembly through metal coordination and/or O₂ activation

03:30pm - 03:55pm USA / Canada - Pacific - April 13, 2021

[Heather Lucas, Presenter](#)

Concluding Remarks

03:55pm - 04:00pm USA / Canada - Pacific - April 13, 2021

Tuesday

Gabor A. Somorjai Award for Creative Research in Catalysis (2021): Symposium honoring Paul J Chirik:

01:00pm - 04:00pm USA / Canada - Pacific - April 13, 2021

[Tianning Diao, Organizer](#) | [Tyler Pabst, Presider](#)

Tuesday

Preparing chemical vapor deposition precursors and polysilazanes through manganese catalysis

01:00pm - 01:25pm USA / Canada - Pacific - April 13, 2021

[Thu Thao Nguyen](#) | [Tufan Mukhopadhyay](#) | [Ryan Trovitch, Presenter](#)

New organometallic strategies for the synthesis of polyesters

01:25pm - 01:50pm USA / Canada - Pacific - April 13, 2021

[Ian Tonks, Presenter](#)

Redox-activity of pyridine-oxazoline ligands in the stabilization of organometallic nickel(I) complexes

01:50pm - 02:15pm USA / Canada - Pacific - April 13, 2021

[Tianning Diao, Presenter](#)

Tuesday

Intermission

02:15pm - 02:25pm USA / Canada - Pacific - April 13, 2021

Tuesday

Iron catalyzed synthesis and chemical recycling of telechelic, 1,3-enchaind oligocyclobutanes

02:25pm - 02:45pm USA / Canada - Pacific - April 13, 2021

[Megan Mohadjer Beromi, Presenter](#)

Role of push-pull proton shuttles in catalytic amide hydrogenation

02:45pm - 03:10pm USA / Canada - Pacific - April 13, 2021

[Lluis Suarez](#) | [Upul Jayarathne](#) | [Nilay Hazari](#) | [Ainara Nova](#) | [Wesley Bernskoetter, Presenter](#)

[Process development for 2'-F-adenosine-5'-monothiophosphat](#)

03:10pm - 03:35pm USA / Canada - Pacific - April 13, 2021

[Jennifer Obligacion, Presenter](#)

[Cyclic voltammetry as a probe of electronic environment at nanomaterial catalyst interfaces](#)

03:35pm - 04:00pm USA / Canada - Pacific - April 13, 2021

[Brandi Cossairt, Presenter](#) | [Ding-Yuan Kuo](#) | [Micaela Homer](#)

Tuesday

[National Fresenius Award \(2020\): Symposium Honoring Kyle M, Lancaster:](#)

01:00pm - 04:00pm USA / Canada - Pacific - April 13, 2021

[Jonathan Caranto, Organizer, Presider](#)

Track: [INOR] Division of Inorganic Chemistry

Division/Committee: [INOR] Division of Inorganic Chemistry

Tuesday

[Introductory Remarks](#)

01:00pm - 01:05pm USA / Canada - Pacific - April 13, 2021

Track: [INOR] Division of Inorganic Chemistry

Tuesday

[Electrocatalytic nitrite reduction to hydroxylamine and ammonium in neutral water](#)

01:05pm - 01:25pm USA / Canada - Pacific - April 13, 2021

[Prof. Kara L. Bren, Presenter](#) | [Jesse R. Stroka](#) | [Ellen Matson](#) | [Yixing Guo](#) | [Banu Kandemir](#)

[Transition metal-mediated N-N coupling reactions and implications for organocatalytic ammonia oxidation at low overpotential](#)

01:25pm - 01:45pm USA / Canada - Pacific - April 13, 2021

[James Gerken, Presenter](#) | [Fei Wang](#) | [Shannon Stahl](#)

[Iron complexes of a new SCS pincer ligand](#)

01:45pm - 02:05pm USA / Canada - Pacific - April 13, 2021

[Kazimer Skubi](#) | [Reagan Hooper](#) | [Melissa Bollmeyer](#) | [Brandon Mercado](#) | [Samantha Macmillan](#) | [Kyle Lancaster](#) | [Patrick Holland, Presenter](#)

[High-valent chemistry with metal-metal bonded compounds: Efforts toward a nitrogen economy](#)

02:05pm - 02:25pm USA / Canada - Pacific - April 13, 2021

[John Berry, Presenter](#)

[Discussion](#)

02:25pm - 02:40pm USA / Canada - Pacific - April 13, 2021

[Activation of O₂ and NO at nonheme, mononuclear, sulfur-ligated iron centers](#)

02:40pm - 03:00pm USA / Canada - Pacific - April 13, 2021

[David Goldberg, Presenter](#) | [Jesse Gordon](#) | [Alex Confer](#) | [Aniruddha Dey](#)

[Are Reductive Eliminations from Organocopper Species Reductive? A Valence Bond Study of \(CuR₄\)⁻ \(R = CH₃ or CF₃\)](#)

03:00pm - 03:20pm USA / Canada - Pacific - April 13, 2021

[Jason Shearer, Presenter](#)

[Microbial strategies for production of cis,cis-muconic acid from lignin biomass](#)

03:20pm - 03:40pm USA / Canada - Pacific - April 13, 2021

[Avery Vilbert, Presenter](#) | [Wayne Kontur](#) | [Jose Perez](#) | [Daniel Noguera](#) | [Timothy Donohue](#)

[The CYP homolog TxtE resists reduction of the {FeO₂}₈ intermediate, promoting efficient Trp nitration](#)

03:40pm - 04:00pm USA / Canada - Pacific - April 13, 2021

[Jonathan Caranto, Presenter](#) | [Christopher Martin](#) | [Manyun Chen](#) | [Maria Martinez](#) | [Yousong Ding](#)

Tuesday

[Chemistry of Materials: Metal Organic Frameworks:](#)

01:00pm - 03:40pm USA / Canada - Pacific - April 13, 2021

[Claus Lugmair, Organizer](#) | [Dr. Alexander Samokhvalov, Presider](#) | [Sourav Saha, Presider](#)

Tuesday

[Effects of confinement on the photophysics of Zn\(II\) phthalocyanine tetrasulphonic acid and Zn\(II\) tetra\(4-sulphonatophenyl\)porphyrin encapsulated within the pores of HKUST-1\(Zn\)](#)

01:00pm - 01:20pm USA / Canada - Pacific - April 13, 2021

[Dr Randy W. Larsen, Presenter](#) | [Lukasz Wojtas](#)

[Competitive adsorption and reactive chemical species identification in RE-DOBDC MOFs via AIMD](#)

01:20pm - 01:40pm USA / Canada - Pacific - April 13, 2021

[Dayton Vogel, Presenter](#) | [Tina Nenoff](#) | [Jessica Rimsza](#)

[Electrically conductive 3D metal-organic framework featuring \$\pi\$ -acidic hexaazatriphenylene hexacarbonitrile ligands with anion- \$\pi\$ interaction and efficient charge-transport capabilities](#)

01:40pm - 02:00pm USA / Canada - Pacific - April 13, 2021

[Ashok Yadav, Presenter](#) | [Dillip Panda](#) | [Shiyu Zhang](#) | [Wei Zhou](#) | [Sourav Saha](#)

[Controlled growth and self-assembly mechanism of the millimeter-sized non-centrosymmetric Zn\(3-ptz\)₂ MOF single crystal](#)

02:00pm - 02:20pm USA / Canada - Pacific - April 13, 2021

[Juan Manuel Garcia, Presenter](#) | [Ignacio Chin](#) | [Javier Enríquez](#) | [Leonardo Vivas](#) | [Federico J. Henández](#) | [Iván Jara](#) | [Felipe Herrera](#) | [Singh Dinesh Pratap](#)

[Unusual highly hygroscopic Al-MOF MIL-160\(Al\): Synthesis, purification, advanced spectroscopic characterization, and kinetics of water sorption by in-situ FTIR and gravimetric measurements](#)

02:20pm - 02:40pm USA / Canada - Pacific - April 13, 2021

[Barrington D. Henry Jr.](#) | [Dr. Alexander Samokhvalov, Presenter](#)

[Opening the black box: New strategies for the synthesis of metal-organic frameworks](#)

02:40pm - 03:00pm USA / Canada - Pacific - April 13, 2021

[Zihao Wang](#) | [Marcus Ng](#) | [Zongzhe Li](#) | [Luc Wetherbee](#) | [Tristan Pitt](#) | [Mickayla Smith](#) | [José J. Fuentes-Rivera](#) | [Arjun Halder](#) | [David Baine](#) | [Jung-Hoon Lee](#) | [Alexander Forse](#) | [Phillip Milner, Presenter](#)

[Biocompatible metal-organic frameworks for the storage and therapeutic delivery of hydrogen sulfide](#)

03:00pm - 03:20pm USA / Canada - Pacific - April 13, 2021

[Ruth Mandel, Presenter](#) | [Faith Chen](#) | [Joshua Woods](#) | [Jung-Hoon Lee](#) | [Jesse Hsu](#) | [José J. Fuentes-Rivera](#) | [Justin Wilson](#) | [Phillip Milner](#)

[Intervalence charge transfer interaction in electrically conducting 3D metal-organic frameworks containing \$\pi\$ -stacked mixed-valent tetrathiafulvalene ligands](#)

03:20pm - 03:40pm USA / Canada - Pacific - April 13, 2021

[Sourav Saha, Presenter](#) | [Shiyu Zhang](#) | [Ashok Yadav](#) | [Dillip Panda](#)

Track: [INOR] Division of Inorganic Chemistry

Tuesday

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

05:00pm - 07:40pm USA / Canada - Pacific - April 13, 2021

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

Tuesday

[Strategies toward highly efficient perovskite solar cells](#)

05:00pm - 05:25pm USA / Canada - Pacific - April 13, 2021

[Yang Yang, Presenter](#)

Tuesday

[The materials science of halide perovskites and solar cells](#)

05:25pm - 05:50pm USA / Canada - Pacific - April 13, 2021

[Prof. Nitin P. Padture, Presenter](#)

[Resonant infrared, matrix-assisted pulsed laser evaporation of hybrid organic-inorganic perovskites: A new thin-film deposition technique for a new semiconductor technology](#)

05:50pm - 06:15pm USA / Canada - Pacific - April 13, 2021

[Adrienne Stiff-Roberts, Presenter](#) | [Niara Wright](#)

[Discussion](#)

06:15pm - 06:25pm USA / Canada - Pacific - April 13, 2021

Tuesday

[Stable and safe perovskite solar cells by sulfur-equipped metal-organic frameworks](#)

06:25pm - 06:50pm USA / Canada - Pacific - April 13, 2021

[Zhengtao Xu, Presenter](#) | [Zonglong Zhu](#) | [Alex K.-Y. Jen](#)

[Vacuum processed halide perovskite light emitting diodes](#)

06:50pm - 07:15pm USA / Canada - Pacific - April 13, 2021

[Jiang Tang, Presenter](#)

[Organic-to-inorganic structural chirality transfer in 2D hybrid perovskites and impact on Rashba-Dresselhaus spin-orbit coupling](#)

07:15pm - 07:40pm USA / Canada - Pacific - April 13, 2021

[Manoj Kumar Jana, Presenter](#) | [Ruyi Song](#) | [Haoliang Liu](#) | [Dipak Raj Khanal](#) | [Svenja Janke](#) | [Rundong Zhao](#) | [Chi Liu](#) | [Yi Xie](#) | [Pete Sercel](#) | [Z. Vally Vardeny](#) | [Volker Blum](#) | [David Mitzi](#)

Tuesday

Chemistry of Materials: Metal Organic Frameworks:

05:00pm - 07:40pm USA / Canada - Pacific - April 13, 2021

[Claus Lugmair, Organizer](#) | [Dayton Vogel, Presider](#) | [Qiang Zhang, Presider](#)

Tuesday

Molecular control and mechanistic insight of modulated MOF particle growth

05:00pm - 05:20pm USA / Canada - Pacific - April 13, 2021

[Carl Brozek, Presenter](#) | [Checkers Marshall](#)

Transition- metal complexes for C-H activation reactions to construct valuable C-N bonds through nitrene-transfer chemistry

05:20pm - 05:40pm USA / Canada - Pacific - April 13, 2021

[Meenakshi Sharma, Presenter](#)

Advent of electrically conducting double-helical metal-organic frameworks featuring butterfly-shaped electron rich π -extended tetrathiafulvalene ligands

05:40pm - 06:00pm USA / Canada - Pacific - April 13, 2021

[Monica Gordillo Varela, Presenter](#) | [Paola Benavides](#) | [Dillip Panda](#) | [Sourav Saha](#)

Post-synthetic installation of redox-active interstitials form extended conductivity pathways in metal-organic frameworks: insights from electronic structure theory and statistical models

06:00pm - 06:20pm USA / Canada - Pacific - April 13, 2021

[Austin Mroz, Presenter](#) | [Nick D'Antona](#) | [Christopher Hendon](#)

Highly efficient desulfurization using Zr-based MOFs

06:20pm - 06:40pm USA / Canada - Pacific - April 13, 2021

[Leiduan Hao](#) | [Lydia Weddle](#) | [Qiang Zhang, Presenter](#)

Preferential binding of SO_x versus H₂O in Mg-MOF-74 from a humid gas stream

06:40pm - 07:00pm USA / Canada - Pacific - April 13, 2021

[Susan Henkelis, Presenter](#) | [Patrick Judge](#) | [Prof. Sophia E. Hayes](#) | [Tina Nenoff](#)

Ab initio molecular dynamics of isotope separation in porous organic cages

07:00pm - 07:20pm USA / Canada - Pacific - April 13, 2021

[Dayton Vogel, Presenter](#) | [Jessica Rimsza](#) | [Tina Nenoff](#)

Solvent-free and phase-selective synthesis of aluminum-trimesate metal-organic frameworks

07:20pm - 07:40pm USA / Canada - Pacific - April 13, 2021

[Jiahong Li, Presenter](#)

Tuesday

Inorganic Spectroscopy:

05:00pm - 08:00pm USA / Canada - Pacific - April 13, 2021

[Dr. Codrina Popescu, Organizer, Presider](#) | [Dr. Alexander Samokhvalov, Presider](#)

Tuesday

[Structure and dynamics of complex oxyfluorides through the lens of solid-state NMR spectroscopy](#)

05:00pm - 05:20pm USA / Canada - Pacific - April 13, 2021

[Dr. Kent J. Griffith, Presenter](#) | [Matthew Nisbet](#) | [Fenghua Ding](#) | [Yiran Wang](#) | [Can Koçer](#) | [Andrew Morris](#) | [Kenneth Poeppelmeier](#)

[TD-DFT photophysical properties simulation of d8 nickel\(II\) qubit candidates.](#)

05:20pm - 05:40pm USA / Canada - Pacific - April 13, 2021

[Domllermut Alamo, Presenter](#) | [Thomas Cundari](#)

[Spectroscopic studies of magnetic transitions and spin-phonon couplings in Co-based single-molecule magnets](#)

05:40pm - 06:00pm USA / Canada - Pacific - April 13, 2021

[Alexandria N. Bone, Presenter](#) | [Chelsea Widener](#) | [Duncan Moseley](#) | [Zhiming Liu](#) | [Zhengguang Lu](#) | [Yongqiang Cheng](#) | [Luke Daemen](#) | [Mykhaylo Ozerov](#) | [Komalavalli Thirunavukkuarasu](#) | [Dmitry Smirnov](#) | [Samuel Greer](#) | [Stephen Hill](#) | [Jurek Krzystek](#) | [Joshua Telser](#) | [Kim Dunbar](#) | [Ziling Xue](#)

[Lanthanide doped upconverting nanoparticles for in vivo imaging of intraluminal pressure dynamics](#)

06:00pm - 06:20pm USA / Canada - Pacific - April 13, 2021

[Jason Casar, Presenter](#) | [Jennifer Dionne](#) | [Miriam Goodman](#) | [Chris Siefe](#) | [Alice Lay](#) | [Claire McLellan](#)

[Applications of \$\beta\$ -NMR spectroscopy in inorganic chemistry](#)

06:20pm - 06:40pm USA / Canada - Pacific - April 13, 2021

[Dr. Monika Stachura, Presenter](#) | [Daniel Szunyogh](#) | [Lars Hemmingsen](#) | [Andrew Macfarlane](#) | [Peter Thulstrup](#)

[Time-resolved infrared spectroscopy of \[FeFe\]-hydrogenase model compounds](#)

06:40pm - 07:00pm USA / Canada - Pacific - April 13, 2021

[Dr. Christopher Stromberg, Presenter](#) | [Edwin Heilweil](#)

[High-resolution solid-state synchronous fluorescence spectroscopy of metal-organic frameworks and their complexes](#)

07:00pm - 07:20pm USA / Canada - Pacific - April 13, 2021

[Cole Grinnell](#) | [Dr. Alexander Samokhvalov, Presenter](#)

[Electronic structures of Cr³⁺ and V²⁺ polypyridyl systems: Undertones in an isoelectronic \(d³\) analogy](#)

07:20pm - 07:40pm USA / Canada - Pacific - April 13, 2021

[Justin Joyce, Presenter](#) | [Romeo Portillo](#) | [Matthew Shores](#) | [Anthony Rappe](#)

[Electronic structure studies of cationic boron formazanate complexes](#)

07:40pm - 08:00pm USA / Canada - Pacific - April 13, 2021

[Benji Katzman, Presenter](#) | [Ryan Maar](#) | [Paul Boyle](#) | [Viktor Staroverov](#) | [Joe Gilroy](#)

Tuesday

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

05:00pm - 06:40pm USA / Canada - Pacific - April 13, 2021

[Nora Radu, Organizer](#) | [Wesley Farrell, Presider](#)

Tuesday

Decomposition of vanadium(V) alkylidenes relevant to olefin metathesis

05:00pm - 05:20pm USA / Canada - Pacific - April 13, 2021

Wesley Farrell, Presenter

Systematic evaluation of the electronic effect of aluminum-containing ligands in iridium-aluminum and rhodium-aluminum bimetallic complexes

05:20pm - 05:40pm USA / Canada - Pacific - April 13, 2021

Natalie Taylor, Presenter

Analysis of the concerted metalation-deprotonation in earth abundant 3d-transition-metal mediated C-H activations

05:40pm - 06:00pm USA / Canada - Pacific - April 13, 2021

William Grumbles, Presenter | **Kortney Melancon** | **Thomas Cundari**

Bisoxazoline-pincer ligated cobalt-catalyzed hydrogenation of alkenes

06:00pm - 06:20pm USA / Canada - Pacific - April 13, 2021

Mikhaila Ritz, Presenter | **William Jones**

Blue light photochemistry in alkyne trimerization at a zirconium center

06:20pm - 06:40pm USA / Canada - Pacific - April 13, 2021

Phuong Minh N. Do, Presenter | **Carsten Milsmann**

Track: [INOR] Division of Inorganic Chemistry