

Electronic Structure Contributions to Function (Celebrating Edward Solomon, Stanford)

Organizers: Peng Chen, Abhishek Dey, and Ryan Hadt
August 25-26, 2026

Tuesday AM

McCormick Place Convention Center W184bc
R. Hadt and L. Quintanar, *Presiding*

8:00 AM. Modulating copper enzymatic activity by tuning secondary coordination sphere interactions. **Y. Lu**

8:30 AM. Insights into the bioinorganic chemistry of Alzheimer's and cataracts disease.
L. Quintanar

9:00 AM. Linking the ATP and allosteric sites in EGFR: Applying a bioinorganic mindset as a medicinal chemist. **D. Heppner**

9:30 AM. Illuminating the cell biology of zinc. **A.E. Palmer**

10:00 AM. Intermission.

10:30 AM. Ultrafast spin coherence in molecules and metalloproteins. **R. Hadt**

11:00 AM. Using XAS to probe the electronic origins of spin relaxation in molecular qubits.
J. Zsombor-Pindera, N. Kazmierczak, R. Hadt, **P. Kennepohl**

11:30 AM. UV-Vis-NIR magnetic circular and linear dichroism spectroscopies for f-block electronic structure. **W.J. Transue**, S. Giles, K. O'Neil, I. Ramsier

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Tuesday PM

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P. Chen and M. L. Kirk, *Presiding*

2:00 PM. Outer sphere thermodynamic contributions to the affinity of proteins for metal ions. **D. Wilcox**

2:30 PM. Electronic structure contributions of sulfido ligation to catalysis in Mo and W enzymes. **M.L. Kirk**

3:00 PM. Cobalt-carbon bond cleavage: spectroscopic insights into cobalamin chemistry. **J.E. Penner-Hahn**, R.J. Sension, S. Berry, N. Ghodrati, B. Van Kuiken

3:30 PM. Intermission.

4:00 PM. Illuminating the methane oxidation cycle in copper zeolites with spectroscopy. D. Plessers, A. Heyer, J. Ma, H.M. Rhoda, M.L. Bols, R.A. Schoonheydt, E.I. Solomon, **B.F. Sels**

4:30 PM. Tuning color centers in nanodiamonds with surface chemistry. **A. Braun**, J.S. Owen

5:00 PM. Copper–oxyl intermediates that convert methane into methanol. **B.E. Snyder**, S. Sur, A. Norris

5:30 PM. Super-resolution imaging of catalysis: From fluorescent to nonfluorescent reactions. **P. Chen**

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J. Kovacs, S. Tian, *Presiding*

8:00 AM. Proton coupled electron transfer to heme ferrous dioxygen and nitrosyl adducts.
A. Dey

8:30 AM. The activation of nitric oxide by diiron complexes: The role of redox potential and hydrogen bonding. **N. Lehnert**

9:00 AM. Formation and spectroscopic characterization of a non-heme Fe^{III}-OOH semiquinonate intermediate. **T. Ohta**, R. Masui, T. Yoshikawa, T. Takeyama, Y. Ohki, Y. Kobayashi, S. Kitao, M. Seto

9:30 AM. Copper coordination chemistry with hindered hydrotris(pyrazolyl)borates: Collaborations with Professor Ed Solomon. **K. Fujisawa**

10:00 AM. Intermission.

10:30 AM. Sigma non-innocence contributions to organonickel photoreactions and small molecule activation. **K. Park**

11:00 AM. Thermodynamic principles behind H-atom abstraction mechanisms and reactivities. **M. Srnec**, Z. Wojdyla, J. Chalupský, J. Gopinath

11:30 AM. Experiment/theory 'entanglement' revealed a conclusive mechanistic picture of the oxygenase/oxidase reaction cycle catalyzed by the coupled bicupric (CBC) active site of tyrosinase: 'en route' to structure/function correlations across CBC family of enzymes.
L. Rulisek, E.I. Solomon, L.D. Elmendorf, A. Stanczak, I. Kipouros, A. Madabeni

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2:00 PM. Targeted discovery and structural basis of a promiscuous non-heme Fe halogenase. **I. Kipouros**, M. Chang

2:30 PM. Hydroquinone 1,2-dioxygenase (PnpC1C2): A platform for enzyme engineering for activity towards novel substrates. **T.E. Machonkin**

3:00 PM. Structural and spectroscopic insights into the radical mechanism of cobalamin-dependent mutases. K. Pham, P. Voss, A.T. Poore, S. Tjia-Fleck, X. Zhang, S. Yachuw, **S. Tian**

3:30 PM. Intermission.

4:00 PM. Thermally and photothermally activated diradicals: From small molecule Bioreagents to nanomedicine applications. **J.M. Zaleski**

4:30 PM. Metal-oxygen intermediates in dioxygen activation and formation reactions. **W. Nam**

5:00 PM. Role of thiolates in creating more reactive iron dioxygen intermediates. **J. Kovacs**, D. Malik, S. Bhatia, M.N. Blakely, H. Bautel

5:30 PM. Metalloenzyme inspired copper(I)-O₂ coordination chemistry. **K.D. Karlin**