

**Chun-Hsing (Josh) Chen, Ph.D.**

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**CAREER & EDUCATION**

**Director, X-ray Crystallography Core Laboratory (XCL) – UNC Chapel Hill      2018 – Present**

Manage the XCL operation at UNC-CH, including routine and non-routine small-molecule single crystal (SC-) X-ray structure determination, X-ray powder diffraction analysis, and other diffraction experiments. Provide instrument training for both SC- and PXRD analysis and teach graduate-level X-ray crystallography lecture and laboratory courses. Contribute to grant applications to acquire new instruments and equipment. Collaborate with UNC CryoEM Core for microcrystal electron diffraction (MicroED) design and implementation, and with ChemMatCARS at Advanced Photon Source, Argonne National Laboratory for micro-crystallography using synchrotron radiation. Participate in the Department-lead STEM outreach effort to promote scientific literacy.

**Research Crystallographer with rank Associate Scientist – IUMSC      2016–2018**

**Research Crystallographer with rank Assistant Scientist – IUMSC      2011–2016**

**Technical Editor – Journal of Chemical Crystallography      2011–2022**

Editorial work including pre-reviewing manuscripts and handling refereed manuscripts. Contributed to upgrades and improved functionality of the web-based Editorial Manager.

**Post-Doctoral Fellow – IUMSC      2010–2011**

**Ph.D., Physical Chemistry/Materials Science – Brandeis University      2004–2010**

Thesis Advisor: Dr. Bruce M. Foxman

Thesis Title “Structure, Solid-State Reactions and Polymorphism of Molecular Crystals”

- Characterized two-phase, topotactic solid-state reactions using X-ray crystallography.
- Synthesized and characterized dihalobis(phosphine)nickel (II) complexes, alkali metal carboxylates, and their polymorphs.
- Recrystallized and characterized three unknown cinnamic acid derivatives, and carried out solid-state [2+2] photocycloaddition via UV irradiation.

**B.S., Organic Chemistry – University of Massachusetts – Dartmouth      1998–2003**

- Carried out photopolymerization using free-radical photoinitiator such as Lucirin<sup>®</sup> TPO-L, and produced metal ion sensors using porphyrin-embedded polymers.
- Studied the kinetics of single/triplet excited state decay on various porphyrin derivatives using a dye laser, and various metal-to-porphyrin adsorption activities using UV/Visible Spectroscopy.
- Synthesized functional *gem*-difluoroallenes using indium-catalyzed reactions.

**EXPERIENCE & INTERESTS**

- Structure determination of new crystalline solids by X-ray diffraction (SC-XRD) and microcrystal electron diffraction (MicroED).
- Microcrystallography by tunable synchrotron radiation.

- Twinning, phase-transitions, MOFs and cage compounds, modulated structures, and crystallographic experiments at non-ambient conditions.
- Solid-state characterization via XRD, texture analysis, thin-film analysis by XRR, and WAXS.
- Characterization of multi-phase topotactic solid-state reactions using X-ray crystallography.
- Development and characterization of potentially thermo- and photo-reactive co-crystal systems.
- Synthesis and sample preparation under non-ambient conditions.
- Crystallographic software such as APEX2, APEX3, APEX4, PLATON, Oxford *CRYSTALS*, SHELX, Olex2, and crystallographically pertinent databases, including CSD, ICSD, PDB, PDF, and Reciprocal Net.
- Maintenance and repair of diffraction systems including Bruker, Rigaku, PANalytical, and Scintag diffractometers.
- Co-lecturing at the School for Synchrotron Crystallography, hosted by ChemMatCARS and Bruker at the APS, Argonne National Laboratory.
- Teaching in graduate level X-ray crystallography course Chem758 at UNC-CH, co-teaching and guest-lecturing graduate level X-ray crystallography course C631 at Indiana University, as well as teaching of general chemistry topics and user-support in crystallographic laboratories (Instructed general and organic chemistry lab courses in University of Massachusetts and Brandeis University, 2000-2006; managed day-to-day X-ray laboratory operations and carried out service structure determinations, 2006-2009, Brandeis.)
- Other analytical and spectroscopic methods, such as  $^{60}\text{Co}$   $\gamma$ -irradiation, UV-Visible Spectroscopy, GC-MS, NMR, FT-IR/Raman, HPLC, Dye-laser.

## SERVICE

- American Crystallographic Association Service Special Interest Group Chair Elect.
- Ad-hoc reviewer for *Acta Crystallographica*, *Journal of Chemical Crystallography*, and *Polyhedron*.
- Mentoring and tutoring graduate and undergraduate students in the science field.

## AFFILIATIONS

- American Crystallographic Association 2009–present
- American Chemical Society 2006–present
- International Union of Crystallography 2006–present

## TRAINING & CONFERENCES

- Bruker/MIT Symposium 2020 (Porous Materials) February 2020
- Bruker/MIT Symposium 2019 (Quantum Crystallography) February 2019
- Bruker/MIT Symposium 2018 (On Their Shoulders) February 2018
- Bruker/MIT Symposium 2017 (Supramolecular Chemistry) February 2017
- Bruker/MIT Symposium 2016 (PXR for the Single Crystal Community) February 2016
- Bruker/MIT Symposium 2015 (Polymorphism and Crystal Engineering) February 2015
- School for Synchrotron Crystallography December 2014
- IUCr 2014 – 23<sup>rd</sup> Congress and General Assembly July 2014
- PANalytical Powder Diffraction Workshop June 2014
- Bruker/MIT Symposium 2014 (Modern Approaches to Structure Solution) February 2014
- Bruker/MIT Symposium 2013 (NMR and X-Ray Diffraction) February 2013
- Departmental Seminar – Inorganic Chemistry Division January 2013
- American Crystallographic Association Annual Meeting & Exposition. July 2012

- Bruker/MIT Symposium 2012 (Metal Organic Frameworks) February 2012
- Bruker/MIT Symposium 2011 (Catalysis for the 21th Century) January 2011
- Bruker/MIT Symposium 2010 (Non-Standard Data Collection Strategies) March 2010
- Bruker/MIT Symposium 2007 (Charge Density and Time-Resolved Studies) February 2007
- American Chemical Society 234<sup>th</sup> National Meeting & Exposition. August 2007
- American Chemical Society 224<sup>th</sup> National Meeting & Exposition. August 2002

## PATENT

1. Lee, Semin; **Chen, Chun-Hsing**; McDonald, Kevin; Flood, Amar. **2014**. Poly-Cyanostilbene Macrocycles. U.S. Patent WO2014127171A1, filed February 13, 2013, and issued August 21, 2014.

## PUBLICATIONS

1. Rodriguez, T. M.; Deegbey, M.; **Chen, C.-H.**, Jakubikova, E.; Dempsey, J. L. Isocyanide Ligands Promote Ligand-to-Metal Charge Transfer Excited States in a Rhenium(II) Complex. *Inorg. Chem.* **2022**, Ahead of print.
2. Farquhar, A. H.; Gardner, K. E. ; Acosta-Calle, S.; Camp, A. M.; **Chen, C.-H.**; Miller, A. J. M. Cation-Controlled Olefin Isomerization Catalysis with Palladium Pincer Complexes. *Organometallics* **2022**, 41(22), 3366-3372.
3. Assaf, E. A. ; Gonell, S.; **Chen, C.-H.**; Miller, A. J. M. Accessing and Photo-Accelerating Low-Overpotential Pathways for CO<sub>2</sub> Reduction: A Bis-Carbene Ruthenium Terpyridine Catalyst. *ACS Catal.* **2022**, 12(20), 12596-12606.
4. de Jesus Cruz, P.; Cassels, W. R.; **Chen, C.-H.**; Johnson, J. S. Doubly stereoconvergent crystallization enabled by asymmetric catalysis. *Science* **2022**, 376(6598), 1224-1230.
5. Beagan, D. M.; Maciulis, N. A.; Pink, M.; Carta, V.; Huerfano, I. J.; Chen, C.-H.; Caulton, K. G. A Redox-Active Tetrazine-Based Pincer Ligand for the Reduction of N-Oxyanions Using a Redox-Inert Metal. *Chem. Eur. J.* **2021**, 27(45), 11676-11681.
6. Cabelof, A. C.; Carta, V.; **Chen, C.-H.**; Pink, M.; Caulton, K. G. Pincers with diverse donors and their interconversion: application to Ni(II). *Z. Anorg. Allg. Chem.* **2021**, 647(14), 1524-1529.
7. Kurtz, D. A.; Dhar, D.; Elgrishi, N.; Kandemir, B.; McWilliams, S. F.; Howland, W. C.; **Chen, C.-H.**; Dempsey, J. L. Redox-Induced Structural Reorganization Dictates Kinetics of Cobalt(III) Hydride Formation via Proton-Coupled Electron Transfer. *J. Am. Chem. Soc.* **2021**, 143(9), 3393-3406.
8. Liu, Y.; Parks, F. C.; Sheetz, E. G.; **Chen, C.-H.**; Flood, A. H. Polarity-Tolerant Chloride Binding in Foldamer Capsules by Programmed Solvent-Exclusion. *J. Am. Chem. Soc.* **2021**, 143(8), 3191-3204.
9. Camp, A. M.; Kita, M. R.; Blackburn, P. T.; Dodge, H. M.; **Chen, C.-H.**; Miller, A. J. M. Selecting Double Bond Positions with a Single Cation-Responsive Iridium Olefin Isomerization Catalyst. *J. Am. Chem. Soc.* **2021**, 143(7), 2792-2800.
10. Huang, T.; Rodriguez, T. M.; Gruninger, C.; Kurtz, D.; Jordan, A. M.; **Chen, C.-H.**; Dempsey, J. L. Electrochemistry-enabled organometallic transformation: A Case Study of the electrosynthesis of cyclopentadienyl rhenium hydride complexes. *Organometallics* **2020**, 39, 10, 1730-1743.
11. Shang, Wen ; Schlam, Roxana F. ; Hickey, M. B.; Zhou, J.; Wheeler, K. A. ; Diaz de Delgado, G. C. ; **Chen, C.-H.**; Snider, B. B. ; Foxman, B. M. Chemo- and Stereospecific Solid-State Thermal Dimerization of Sodium trans-2-Butenoate and  $\gamma$ -Ray-Induced Single-Crystal-to-Single-Crystal Dimerization of Hexaaquamagnesium trans-2-Butenoate Dihydrate: Both Give rel-(3S,4R)-1-Hexene-3,4-dicarboxylate but by Different Mechanisms. Stereospecific  $\gamma$ -Ray-Induced Trimerization of Sodium trans-2-Butenoate. *Crys. Growth Des.* **2021**, 21(1), 663-682.
12. Dodge, H. M.; Kita, M. R.; **Chen, C.-H.**; Miller, A. J. M. Identifying and Evading Olefin Isomerization Catalyst Deactivation Pathways Resulting from Ion-Tunable Hemilability. *ACS Catal.* **2020**, 10(21), 13019-13030.

13. Martinez, Jorge L.; Lutz, S. A.; Beagan, D. M.; Gao, X.; Pink, M.; **Chen, C.-H.**; Carta, V.; Moenne-Loccoz, P.; Smith, J. M. Stabilization of the Dinitrogen Analogue, Phosphorus Nitride. *ACS Cent. Sci.* **2020**, 6(9), 1572-1577.
14. Lutz, S. A.; Hickey, A. K.; Gao, Y.; **Chen, C.-H.**; Smith, J. M. Two-State Reactivity in Iron-Catalyzed Alkene Isomerization Confers  $\sigma$ -Base Resistance. *J. Am. Chem. Soc.* **2020**, 142(36), 15527-15535.
15. Benson, C. R.; Kacenauskaitė, L.; VanDenburgh, K. L.; Zhao, W.; Qiao, B.; Sadhukhan, T.; Pink, M.; Chen, J.; Borgi, S.; **Chen, C.-H.**; et al. Plug-and-Play Optical Materials from Fluorescent Dyes and Macrocycles. *Chem.* **2020**, 6(8), 1978-1997.
16. Cabelof, A. C.; Carta, V.; **Chen, C.-H.**; Caulton, K. G. Nitrogen oxyanion reduction by Co(II) augmented by a proton responsive ligand: recruiting multiple metals. *Dalton Trans.* **2020**, 49(23), 7891-7896.
17. Huang, T.; Rodriguez, T. M.; Gruninger, C. T.; Kurtz, D. A. ; Jordan, A. M.; **Chen, C.-H.**; Dempsey, J. L. Electrosynthetic Route to Cyclopentadienyl Rhenium Hydride Complexes Enabled by Electrochemical Investigations of their Redox-Induced Formation. *Organometallics* **2020**, 39(10), 1730-1743.
18. Sorsche, D; Miehl, M. E. ; Searles, K.; Gouget, G.; Zolnhofer, E. M.; Fortier, S.; **Chen, C.-H.**; Gau, M.; Carroll, P. J.; Murray, C. B.; et al. Unusual Dinitrogen Binding and Electron Storage in Dinuclear Iron Complexes. *J. Am. Chem. Soc.* **2020**, 142(18), 8147-8159.
19. Rajesh, U. C.; Losovyj, Y.; **Chen, C.-H.**; Zaleski, J. M. Designing Synergistic Nanocatalysts for Multiple Substrate Activation: Interlattice Ag-Fe<sub>3</sub>O<sub>4</sub> Hybrid Materials for CO<sub>2</sub>-Inserted Lactones. *ACS Catal.* **2020**, 10(5), 3349-3359.
20. Valdez-Moreira, J. A.; Millikan, S. P.; Gao, X.; Carta, V.; **Chen, C.-H.**; Smith, J. M. Hydrosilylation of an Iron(IV) Nitride Complex. *Inorg. Chem.* **2020**, 59(1), 579-583.
21. Bruch, Q. J. ; Connor, G. P. ; **Chen, C.-H.**; Holland, P. L. ; Mayer, J. M. ; Hasanayn, F.; Miller, A. J. M. Dinitrogen Reduction to Ammonium at Rhenium Utilizing Light and Proton-Coupled Electron Transfer. *J. Am. Chem. Soc.* **2019**, 141(51), 20198-20208.
22. Smith, J. B.; Camp, Andrew M.; Farquhar, Alexandra H.; Kerr, S. H.; **Chen, C.-H.**; Miller, Alexander J. M. Organometallic Elaboration as a Strategy for Tuning the Supramolecular Characteristics of Aza-Crown Ethers. *Organometallics* **2019**, 38(22), 4392-4398.
23. Cook, B. J.; **Chen, C.-H.**; Pink, M.; Caulton, K. G. Gross rearrangement of Fe(II) aggregate structure by replacement of two H<sup>+</sup> by two Li<sup>+</sup>: Visualizing altered structure of acid versus conjugate base. *Polyhedron* **2019**, 174, 114152.
24. Valdez-Moreira, Juan A.; Thorarinsdottir, Agnes E. ; DeGayner, J. A.; Lutz, S. A.; **Chen, C.-H.**; Losovyj, Y.; Pink, M.; Harris, T. D.; Smith, J. M. Strong  $\pi$ -Backbonding Enables Record Magnetic Exchange Coupling Through Cyanide. *J. Am. Chem. Soc.* **2019**, 141(43), 17092-17097.
25. Lindley, B. M.; Walden, A. G.; Brasacchio, A. M.; Casuras, A.; Lease, N.; **Chen, C.-H.**; Goldman, Alan S.; Miller, A. J. M. Electrochemical C-H bond activation via cationic iridium hydride pincer complexes. *Chem. Sci.* **2019**, 10(40), 9326-9330.
26. Liu, Y.; Zhao, W.; **Chen, C.-H.**; Flood, A. H. Chloride capture using a C-H hydrogen-bonding cage. *Science* **2019**, 365(6449), 159-161.
27. Xu, S.; Kwon, H.-Y.; Ashley, D. C. ; **Chen, C.-H.**; Jakubikova, E.; Smith, J. M. Intramolecular Hydrogen Bonding Facilitates Electrocatalytic Reduction of Nitrite in Aqueous Solutions. *Inorg. Chem.* **2019**, 58(14), 9443-9451.
28. Labrum, N. S. ; **Chen, C.-H.**; Caulton, K. G. A bis-Pyrazolate Pincer on Reduced Cr Deoxygenates CO<sub>2</sub>: Selective Capture of the Derived Oxide by Cr(II). *Chem. Eur. J.* **2019**, 25(33), 7935-7940.
29. Cook, B. J.; Lord, R. L.; **Chen, C.-H.**; Caulton, K. G. Gauging the Redox Non-Innocence of a Highly Pi-Acidic Bis-Tetrazine Pincer Ligand. *Eur. J. Inorg. Chem.* **2019**, 2019(20), 2535-2542.
30. Labrum, N. S.; Pink, M.; **Chen, C.-H.**; Caulton, K. G. Reactivity of an Unusual Divalent Chromium Aggregate Supported by a Multifunctional Bis(pyrazolate) Pincer Ligand. *Eur. J. Inorg. Chem.* **2019**, 2019(14), 1932-1940.

31. Cook, B. J.; Pink, M.; **Chen, C.-H.**; Caulton, K. G. Electrophile Recruitment as a Structural Element in Bis-Pyrazolate Pyridine Complex Aggregation. *Eur. J. Inorg Chem.* **2018**, 2018(48), 5160-5166.
32. Labrum, N. S.; Seo, J.; **Chen, C.-H.**; Pink, M.; Beagan, D. M.; Caulton, K. G. Di- and trivalent chromium bis(pyrazol-3-yl)pyridine pincer complexes with good leaving groups. *Inorganica Chim. Acta* **2019**, 486, 483-491.
33. Seo, J.; Cabelof, A. C.; **Chen, C.-H.**; Caulton, K. G. Selective deoxygenation of nitrate to nitrosyl using trivalent chromium and the Mashima reagent: reductive silylation. *Chem. Sci.* **2019**, 10(2), 475-479.
34. Labrum, N. S.; **Chen, C.-H.**; Caulton, K. G. A new face for bis(pyrazol-3-yl)pyridine: Incompatible geometric preferences dictates unprecedented pincer ligand connectivity. *Inorg. Chim. Acta* **2019**, 485, 54-57.
35. Maciulis, N. A.; Schaugaard, R. N.; Losovyj, Y.; **Chen, C.-H.**; Pink, M.; Caulton, K. G. Seeking Redox Activity in a Tetrazinyl Pincer Ligand: Installing Zerovalent Cr and Mo. *Inorg. Chem.* **2018**, 57(20), 12671-12682.
36. Martinez, J. L.; Lee, W.-T.; Pink, M.; **Chen, C.-H.**; Smith, J. M. Heteroleptic nickel complexes of a bulky bis(carbene)borate ligand. *Polyhedron* **2018**, 156, 297-302.
37. A multimetal-ligand cooperative approach to CO<sub>2</sub> activation By: Cook, B. J.; Polezhaev, A. V.; **Chen, C.-H.**; Pink, M.; Caulton, K. G. *Inorganica Chim. Acta* **2018**, 483, 510-515.
38. Xu, S.; Ashley, D. C.; Kwon, H.-Y.; Ware, G. R.; **Chen, C.-H.**; Losovyj, Y.; Gao, X.; Jakubikova, E.; Smith, J. M. A flexible, redox-active macrocycle enables the electrocatalytic reduction of nitrate to ammonia by a cobalt complex. *Chem. Sci.* **2018**, 9(22), 4950-4958.
39. Cook, B. J.; **Chen, C.-H.**; Caulton, K. G. A Multifunctional Pincer Ligand for Cobalt-Promoted Oxidation by N<sub>2</sub>O. *Chem. Eur. J.* **2018**, 24(22), 5962-5966.
40. Polezhaev, A. V.; Beagan, D. M.; Cabelof, A. C.; **Chen, C.-H.**; Caulton, K. G. A substituent-tolerant synthetic approach to N/P-"loaded" heteroarenes. *Dalton Trans.* **2018**, 47(17), 5938-5942.
41. Lin, H.-J.; Lutz, S.; O'Kane, C.; Zeller, M.; **Chen, C.-H.**; Al Assil, T.; Lee, W.-T. Synthesis and characterization of an iron complex bearing a hemilabile NNN-pincer for catalytic hydrosilylation of organic carbonyl compounds. *Dalton Trans.* **2018**, 47(10), 3243-3247.
42. Zahran, E. M.; Fatila, E. M.; **Chen, C.-H.**; Flood, A. H.; Bachas, L. G. Cyanostar: C-H Hydrogen Bonding Neutral Carrier Scaffold for Anion-Selective Sensors. *Anal. Chem.* **2018**, 90(3), 1925-1933.
43. Cook, B. J.; **Chen, C.-H.**; Pink, M.; Caulton, K. G. Dehydrohalogenation of proton responsive complexes: versatile aggregation via pyrazolate pincer ligand arms. *Dalton Trans.* **2018**, 47(6), 2052-2060.
44. Polezhaev, A. V.; Liss, C. J.; Telser, J.; **Chen, C.-H.**; Caulton, K. G. A PNNH Pincer Ligand Allows Access to Monovalent Iron. *Chem. Eur. J.* **2018**, 24(6), 1330-1341.
45. Xu, S.; Bucinsky, L.; Breza, M.; Krzystek, J.; **Chen, C.-H.**; Pink, M.; Telser, J.; Smith, J. M. Ligand Substituent Effects in Manganese Pyridinophane Complexes: Implications for Oxygen-Evolving Catalysis. *Inorg. Chem.* **2017**, 56(22), 14315-14325.
46. Martinez, J. L.; Lin, H.-J.; Lee, W.-T.; Pink, M.; **Chen, C.-H.**; Gao, X.; Dickie, D. A.; Smith, J. M. Cyanide Ligand Assembly by Carbon Atom Transfer to an Iron Nitride. *J. Am. Chem. Soc.* **2017**, 139(40), 14037-14040.
47. Cook, B. J.; Polezhaev, A. V.; **Chen, C.-H.**; Pink, M.; Caulton, K. G. Deprotonation, Chloride Abstraction, and Dehydrohalogenation as Synthetic Routes to Bis-Pyrazolate Pyridyl Iron(II) Complexes. *Eur. J. Inorg Chem.* **2017**, 2017(34), 3999-4012.
48. Zhao, W.; Qiao, B.; **Chen, C.-H.**; Flood, A. H. High-Fidelity Multistate Switching with Anion-Anion and Acid-Anion Dimers of Organophosphates in Cyanostar Complexes. *Angewandte Chemie, International Edition* **2017**, 56(42), 13083-13087.
49. Baek, S.-Y.; Kurogi, T.; Kang, D.; Kamitani, M.; Kwon, S.; Solowey, D. P.; **Chen, C.-H.**; Pink, M.; Carroll, P. J.; Mindiola, D. J.; et al. Room-Temperature Ring-Opening of Quinoline, Isoquinoline, and Pyridine with Low-Valent Titanium. *J. Am. Chem. Soc.* **2017**, 139(36), 12804-12814.

50. Polezhaev, A. V.; **Chen, C.-H.**; Kinne, A. S.; Cabelof, A. C.; Lord, R. L.; Caulton, K. G. Ligand Design toward Multifunctional Substrate Reductive Transformations. *Inorg. Chem.* **2017**, *56*(16), 9505-9514.
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54. Hickey, A. K.; Lutz, S. A.; **Chen, C.-H.**; Smith, Jeremy M. Two-State Reactivity in C-H Activation by a Four-Coordinate Iron(0) Complex. *Chem. Comm. (Cambridge, United Kingdom)* **2017**, *53*(7), 1245-1248.
55. Hickey, A. K.; Munoz, S. B.; Lutz, S. A.; Pink, M.; **Chen, C.-H.**; Smith, Jeremy M. Arrested  $\alpha$ -hydride migration activates a phosphido ligand for C-H insertion. *Chem. Comm. (Cambridge, United Kingdom)* **2017**, *53*(2), 412-415.
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- Diarylamido-Based PNZ Pincer Ligands: Redox Activity at the Ligand and Donor Ability Toward the Metal. *Inorg. Chem.* **2015**, *54(6)*, 2916-2935.
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