

Curriculum Vitae

Xiongyi Huang, Ph.D.

Assistant Professor of Chemistry

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Professional Experience

- Assistant Professor, Department of Chemistry, Johns Hopkins University (09/2019 – current)

Education

- Postdoctoral Fellow, California Institute of Technology (05/2016 – 09/2019)
Advisor: Prof. Frances Arnold
- Ph.D. in Chemistry, Princeton University (09/2010 – 04/2016)
Advisor: Prof. John T. Groves
- B.S. in Chemistry, University of Science and Technology of China (USTC) (09/2006 – 07/2010)
Advisor: Prof. Yao Fu and Prof. Jing Shi

Research training

- Postdoctoral research with **Prof. Frances Arnold**, Caltech (04/2016 – current)
Utilized evolutionary protein design methods to develop new enzyme catalysts for important chemical transformations not present in nature. This research effort will provide efficient catalysts for chemical synthesis and open up new opportunities for development of new biosynthetic pathways.
- Visiting scholar at **Prof. Ken Houk's** group, UCLA (2017 – current)
Utilized computational modeling tools including molecular dynamics (MD) simulations and quantum mechanics/molecular mechanics (QM/MM) calculations to study the mechanisms of enzymatic catalysis.
- Doctoral thesis research with **Prof. John T. Groves**, Princeton University (09/2010 – 04/2016)
Combined organic synthesis, computational modeling, and inorganic spectroscopies to develop novel C-H functionalization reactions.
- Visiting scientist at **Prof. Jacob Hooker's** group, Mass General Hospital and Harvard Medical School, (07/2013 – 12/2015)
Adapted manganese-catalyzed fluorination reactions for ^{18}F labeling and developed novel imaging agents for disease diagnosis.
- Visiting scientist, **Merck Molecular Imaging Group**, (07/2013 – 12/2015)
Optimized the manganese-based ^{18}F labeling methods for Ci-scale radiolabeling with automated radiosynthesis. Implemented the method for the late-stage ^{18}F labeling of drug candidates.
- Undergraduate thesis research with **Prof. Yao Fu and Jing Shi**, USTC, (01/2008 – 06/2010)
Developed DFT-based computational methods for accurate prediction of molecular properties with high biological and pharmaceutical importance.

Awards and Honors

- 2018 – current NIH Pathway to Independence Award
- 2017 – 2018 NIH Ruth L. Kirschstein Postdoctoral Fellowship
- 2016 Chinese Government Award for Outstanding Students Abroad
- 2013 – 2015 HHMI International Student Research Fellowship

Publications at Caltech

7. Zhang, J.[†]; Huang, X.[†]; Zhang, R. K.; Arnold, F. H.* “Enantiodivergent α -Amino C–H Fluoroalkylation Catalyzed by Engineered Cytochrome P450s”, *J. Am. Chem. Soc.* **2019**, *141*, 9798–9802. (†equal contribution)
6. Huang, X.[†]; Garcia-Borràs, M.[†]; Miao, K.; Kan, S. B. J.; Zutshi, A.; Houk, K. N.*; Arnold, F. H.* “A Biocatalytic Platform for Synthesis of Chiral α -Trifluoromethyl Organoborons”, *ACS Cent. Sci.* **2019**, *5*, 270–276. (†equal contribution) [Featured in [ACS Central Science](#) and [Nature Catalysis](#)]
5. Chen, K.; Huang, X.; Zhang, S. Q.; Zhou, A. Z.; Kan, S. B. J.; Hong, X.*; Arnold, F. H.* “Engineered Cytochrome c-Catalyzed Lactone-Carbene B–H Insertion”, *Synlett.* **2019**, *30*, 378–382.
4. Zhang, R. K.; Chen, K.; **Huang, X.**; Wohlschlager, L.; Renata, H.; Arnold, F. H.* “Enzymatic Assembly of Carbon–Carbon Bonds via Iron-Catalysed sp^3 C–H Functionalization”, *Nature* **2019**, *565*, 67–72. [Selected as the [Nature cover article](#), featured in [Synfacts](#)]
3. Zhang, R. K.; **Huang, X.**; Arnold, F. H.* “Selective C–H Bond Functionalization with Engineered Heme Proteins: New Tools to Generate Complexity”, *Curr. Opin. Chem. Biol.* **2019**, *49*, 67–75.
2. Chen, K.; **Huang, X.**; Kan, S. B. J.; Zhang, R. K.; Arnold, F. H.* “Enzymatic Construction of Highly Strained Carbocycles”, *Science* **2018**, *360*, 71–75. [Featured in [Caltech home page](#), [Phys.org](#), [myScience](#), and [EurekAlert](#)]
1. Kan, S. B. J.[†]; Huang X.[†]; Gumulya, Y.; Chen, K.; Arnold, F. H.* “Genetically Programmed Chiral Organoborane Synthesis”, *Nature* **2017**, *552*, 132–136. (†equal contribution) [Featured in [Caltech News](#), [GEN](#), [myScience](#), [Forbes](#), [ScienceNewsline](#), [EurekAlert](#), [AZoCleantech](#), [Phys.org](#)]

Publications at Princeton

12. Liu, W.; Huang, X.; Placzek, M. S.; Krska, S. W.; McQuade, P.; Hooker, J. M.*; Groves, J. T.* “Site-Selective ^{18}F Fluorination of Unactivated C–H Bonds Mediated by a Manganese Porphyrin”, *Chem. Sci.* **2018**, *9*, 1168–1172.
11. Huang, X.; Groves, J. T.* “Oxygen Activation and Radical Transformations in Heme Proteins”, *Chem. Rev.* **2018**, *118*, 2491–2553.
10. Huang, X.[†]; Zhuang, T.[†]; Kates, P. A.; Gao, X.; Chen, X.; Groves, J. T.* “Alkyl Isocyanates via Manganese-Catalyzed C–H Activation for the Preparation of Substituted Ureas”, *J. Am. Chem. Soc.* **2017**, *139*, 15407–15413. (†equal contribution)
9. Hsieh, C. H.; Huang, X.; Amaya, J. A.; Rutland, C. D.; Keys, C. L.; Groves, J. T.; Austin, R. N.; Makris, T. M. “The Enigmatic P450 Decarboxylase OleT Is Capable of, but Evolved to Frustrate, Oxygen Rebound Chemistry”, *Biochemistry* **2017**, *56*, 3347–3357.
8. Huang, X.; Groves, J. T.* “Beyond Ferryl-Mediated Hydroxylation: 40 Years of the Rebound Mechanism and C–H Activation”, *J. Biol. Inorg. Chem.* **2016**, 1–23.
7. Huang, X.; Groves, J. T.* “Taming Azide Radicals for Catalytic C–H Azidation”, *ACS Catal.* **2016**, *6*, 751–759.
6. Huang, X.; Bergsten, T. M.; Groves, J. T.* “Manganese-Catalyzed Late-Stage Aliphatic C–H Azidation”, *J. Am. Chem. Soc.* **2015**, *137*, 5300–5303.

5. Huang, X.; Liu, W.; Hooker, J. M.; Groves, J. T.* “Targeted Fluorination with the Fluoride Ion by Manganese-Catalyzed Decarboxylation”, *Angew. Chem. Int. Ed.* **2015**, *54*, 5241–5245. [Selected as a “Hot Paper” by Angewandte Chemie]
4. Huang, X.†; Liu, W.†; Ren, H.; Neelamegam, R.; Hooker, J. M.*; Groves, J. T.* “Late Stage Benzylic C–H Fluorination with [¹⁸F]Fluoride for PET Imaging” *J. Am. Chem. Soc.* **2014**, *136*, 6842–6845. (†equal contribution) [Highlighted in C&EN News, *Angew. Chem. Int. Ed.* and *Chem. Sci.*]
3. Liu, W.; Huang, X.; Groves, J. T.* “Oxidative Aliphatic C–H Fluorination with Manganese Catalysts and Fluoride Ion”, *Nat. Protoc.* **2013**, *8*, 2348–2354.
2. Liu, W.; Huang, X.; Cheng, M.; Nielsen, R. J.; Goddard, W. A. III; Groves, J. T.* “Oxidative Aliphatic C–H Fluorination with Fluoride Ion Catalyzed by a Manganese Porphyrin”, *Science* **2012**, *337*, 1322–1325. [Highlighted in *Nature*, C&EN News, *Chemistry World* and *Princeton University home page*]
1. Cooper, H. L. R.; Mishra, G.; Huang, X.; Pender-Cudlip, M.; Austin, R. N.; Shanklin, J.; Groves, J. T.* “Parallel and Competitive Pathways for Substrate Desaturation, Hydroxylation and Radical Rearrangement by the Non-heme Diiron Hydroxylase AlkB”, *J. Am. Chem. Soc.* **2012**, *134*, 20365–20375.

Publications at USTC

4. Shi, J.*; Huang, X.; Wang, H. J.; Fu, Y. “Hydride Dissociation Energies of Six-Membered Heterocyclic Organic Hydrides Predicted by ONIOM-G4 Method”, *J. Chem. Inf. Model.* **2012**, *52*, 63–75.
3. Shi, J.*; Huang, X.; Wang, J. P.; Li, R. “A Theoretical Study on C-COOH Homolytic Bond Dissociation Enthalpies”, *J. Phys. Chem. A* **2010**, *114*, 6263–6272.
2. Huang, X.; Wang, H. J.; Shi, J.* “Theoretical Study on Acidities of (*S*)-Proline Amide Derivatives in DMSO and Its Implications for Organocatalysis”, *J. Phys. Chem. A* **2010**, *114*, 1068–1081.
1. Wang, H.-J.; Huang, X.; Shen, R.; Fu, Y.*; Rui, L. “Theoretical Study of One-Electron Redox Potentials of Some NADH Model Compounds”, *Chin. J. Chem.* **2010**, *28*, 72–80.

Patents

6. Chen, K.; Huang, X.; Jennifer, S.B.J. “Biocatalytic Synthesis of Strained Carbocycles”, World Patent WO2018175628, Sep 27, 2018.
5. Jennifer, S.B.J.; Huang, X.; Chen, K. “Heme Protein Catalysts for Carbon–Boron Bond Formation *In Vitro* and *In Vivo*”, World Patent WO2018165325, Sep 13, 2018.
4. Groves, J.T.; Huang, X. “Targeted, Metal-Catalyzed Fluorination of Complex Compounds with Fluoride Ion via Decarboxylation”, World Patent WO2016130549, Aug 8, 2016.
3. Groves, J.T.; Huang, X. “Direct Oxidative Carbon-Hydrogen Fluorination of a Carbon Containing Compound, Comprises Combining a Carbon Containing Compound, a Fluorinating Agent, a Fluorinating Catalyst, and an Oxidant”, U.S. Patent US20160158388, June 9, 2016.
2. Groves, J.T.; Huang, X.; Liu, W. “Methods and Compositions for Direct Radioactive Labeling of Bio-Active Molecules and Building Blocks”, World Patent WO2015134467, Sep 11, 2015.
1. Groves, J.T.; Liu, W.; Huang, X. “C–Halogen Bond Formation”, World Patent WO2015054476, April 16, 2015.