Curriculum Vitae

Tzuhsiung (Nick) Yang (楊自雄)

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PROFESSIONAL EXPERIENCES

Assistant Professor **Aug 2022—Current**

Department of Chemistry, National Tsing Hua University, Taiwan ROC

Research topic: 1) Generative AI models for Chemistry: small molecule cancer drugs, spintronics, and redox flow battery; 2) Quantum chemical simulations: homogenous catalysis, enzymatic reactions, molecular spin qubits, 3) High throughput virtual screening: molecular spin qubits and organic light emitting diodes (OLED).

Postdoctoral Associate **Sep 2019—Feb 2021**

Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA

Advisor: Prof. Rafael Gomez-Bombarelli

Research topic: *De novo* design of novel organic photodiodes using deep generative models

Postdoctoral Associate **Jun 2018—May 2019**

Department of Chemical Engineering, Massachusetts Institute of Technology, USA

Advisor: Prof. Heather J. Kulik

Research topic: Combining data-mining, high throughput computing, and machine learning to discovery inorganic complexes that are of the potential for single site catalysis

HONORS AND AWARDS

1. MOE Yushan Young Fellowship (2022-2027)

EDUCATION

Ph, D, Chemistry **Jan 2015—May 2018**

University of Wisconsin—Madison

Department of Chemistry

Advisor: Prof. John F. Berry

Thesis: Electronic and steric effect in transition metal catalyzed group transfer reactions: Paving the road to high throughput virtual screening of catalysts

B.S., Chemistry **Sep 2009—May 2013**

University of Wisconsin-Madison

College of Letters and Science, 1305 Linden Drive, Madison, WI 53706 USA

B.S., Biochemistry **Sep 2009—May 2013**

University of Wisconsin-Madison

College of Agriculture and Life Science, 1450 Linden Drive, Madison, WI 53706

PUBLICATIONS

Corresponding publications

1. Lee, Z.-H.; Chen, Y.-T.; Chang, H.-T.; Yang, T.* ChemRxiv, 2023. "A Joint Semi-Supervised Variational Autoencoder and Transfer Learning Model for Designing Molecular Transition Metal Complexes," https://chemrxiv.org/engage/chemrxiv/article-details/6500468299918fe537d199ec

2. Wu, Y.-T.; Kumbhar, S.; Tsai, R.-F.; Yang, Y.-C.; Zeng, W.-Q.; Hsu, W.-C.; Chiang, Y.-W.; Yang, T.;* Lu, I-C.;* Wang, Y.-H.* *ACS Org. Inorg. Au,* **2024***,* 4, 306. "Manipulating the Rate and Overpotential for Enhanced Electrochemical Water Oxidation: Mechanistic Insights for Cobalt Catalysts Bearing Non-innocent Bis(benzimidazole)pyrazolide Ligands"
3. Lee, Z.-H.; Lin, P. C.; Yang, T.* *J. Chin. Chem. Soc.* **2023**, *70 (5)***,** 1095. "Inverse Design of Ligands Using a Deep Generative Model Semi-Supervised by a Data-Driven Ligand Field Strength Metric"
4. Hsu, W.-C.; Zeng, W.-Q.; Lu, I.-C.* Yang, T.;* Wang, Y.-H.* *ChemSusChem.* **2022***,* e202201. "Dinuclear Cobalt Complexes for Homogeneous Water Oxidation: Tuning Rate and Overpotential Through the Redox Non-Innocent Ligand"
5. Yang, T.;* Berry, J. F.* *J. Chem. Theory Comput.* **2018**, *14*, 3459. "Numerical Nuclear Second Derivatives on a Computing Grid: Enabling and Accelerating Frequency Calculations on Complex Molecular Systems"

(Co)First-authored publications

6. Taylor, M. G.;⊥ Yang, T.;⊥ Lin, S.;⊥ Nandy, A.; Janet, J. P.; Duan, C.; Kulik, H. J.* *J. Phys. Chem. A*, **2020**, *124*, 3286. "Seeing is believing: Experimental spin states from machine learning model structure predictions," ⊥**These authors contributed equally**
7. Huang, M.;⊥ Yang, T.;⊥ Paretsky, J.; Berry, J. F.;* Schomaker, J. M.* *J. Am. Chem. Soc.* **2017**, *139*, 17376. "Inverting Steric Effects: Using 'Attractive' Non-Covalent Interactions to Direct Silver- Catalyzed Nitrene Transfer" ⊥**These authors contributed equally**
8. Dolan, N. S.;⊥ Scamp, R. J.;⊥ Yang, T.;⊥ Berry, J. F.;* Schomaker, J. M.* *J. Am. Chem. Soc.* **2016**, *138*, 14658. "Catalyst-Controlled and Tunable, Chemoselective Silver-Catalyzed Intermolecular Nitrene Transfer: Experimental and Computational Studies" ⊥**These authors contributed equally**
9. Yang, T.; Quesne, M. G.; Neu, H. M.; Cantu, F. G.; Goldberg, D. P.;* de Visser, S. P.* *J. Am. Chem. Soc.* **2016**, *138*, 12375. "Singlet versus Triplet Reactivity in an Mn(V)-Oxo Species: Testing Theoretical Predictions Against Experimental Evidence"
10. Varela-Álvarez, A.;⊥ Yang, T.;⊥ Jennings, H.; Kornecki, K. P.; Macmillan, S. N.; Lancaster, K. M.; Mack, J. B. C.; Du Bois, J.; Berry, J. F.;* Musaev, D. G.* *J. Am. Chem. Soc.* **2016**, *138*, 2327. "Rh_2(II,III) Catalysts with Chelating Carboxylate and Carboxamidate Supports: Electronic Structure and Nitrene Transfer Reactivity," ⊥**These authors contributed equally**

Co-authored publications

11. Tseng, C.-C.; Ding, Y.-W.; Chen, Z.-Y.; Lan, H.-Y.; Li, H.-J.; Cheng, Y.-S.; Kuo, T.-S.; Chen, P.-L.; Wu, W.-C.; Shi, F.-K.; Yang, T.; Liu, H.-J. *Inorg. Chem.* **2024**, *63*, 11361 "A Bis-Cyclopentadienyl Ligand-Supported Di-Iron Trihydride Motif as a Synthon for Access to Heterobimetallic Trinuclear Complexes."
12. Subramanian, A.; Greenman, K. P.; Gervaix, A.; Yang, T.; Gómez-Bombarelli, R.* *Digital Discovery,* **2023***, 2,* 1006 "Automated patent extraction powers generative modeling in focused chemical spaces."
13. Ting, J.-H.; Lin, P.-C.; Gupta, S.; Liu, C.-H.; Yang, T.; Lee, C.-Y.; Lai, Y.-T.;* Tai, N.-H.* *Nano. Adv.,* **2023**, *5*, 4881 "Dipole Moment as Underlying Mechanism for Enhancing Immobilization of Glucose Oxidase by Ferrocene-Chitosan for Superior Specificity Non-invasive Glucose Sensing,"
14. Subramanian, A.; Greenman, K. P.; Gervaix, A.; Yang, T.; Gomez-Bombarelli, R.* *Digital Discovery* **2023, *2*,** 1006. "Automated patent extraction powers generative modeling in focused chemical spaces"
15. He, X.; Yang, T.; Iliescu, A.; Arguilla, M. Q.; Chen, T.; Kulik, H. J.; Dincă, M.* *J. Am. Chem. Soc.* **2023**, *145*, 16872. "Reversible O–O Bond Scission and O2 evolution at MOF-supported Tetramanganese Clusters"
16. Park, S. V.; Corcos, A. R.; Jambor, A. N.; Yang, T.; Berry, J. F.* *J. Am. Chem. Soc.* **2022**, *144*, 3259 "Formation of the N≡ N Triple Bond from Reductive Coupling of a Paramagnetic Diruthenium Nitrido Compound"
17. Mohapatra, S.; Yang, T.; Gomez-Bombarelli, R.* *Nat. Mach. Intell.* **2020**, *2*, 749. "Reusability report: Designing organic photoelectronic molecules with descriptor conditional recurrent neural networks"
18. Wang, W.; Yang, T.; Harris, W. H.; Gomez-Bombarelli, R.* *Chem. Comm.,* **2020**, *56*, 8920. "Active learning and neural network potentials accelerate molecular screening of ether-based solvate ionic liquids"
19. Liu, F.; Yang, T.; Yang, J.; Xu, E.; Bajaj, A.; Kulik, H. J.* *Front. Chem.*, **2019**, *7,* 219. "Bridging the Homogeneous-Heterogeneous Divide: Modeling Spin for Reactivity in Single Atom Catalysis"
20. Janet, J. P.; Liu, F.; Nandy, A.; Duan, C.; Yang, T.; Lin, S.; Kulik, H. J.* *Inorg. Chem.*, **2019**, *58,* 10592. "Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry"
21. Janet, J. P.; Duan, C.; Yang, T.; Nandy, A.; Kulik, H. J.* *Chem. Sci.* **2019**, *10*, 7913. "A quantitative uncertainty metric controls error in neural network-driven chemical discovery"
22. Ren, Z.; Sunderland, T. L.; Tortoreto, C.; Yang, T.; Berry, J. F.;* Musaev, D. G.;* Davies, H. M. L.* *ACS Catal.*

2018, *8*, 10676. “Comparison of reactivity and enantioselectivity between chiral bimetallic catalysts: bismuth–rhodium-and dirhodium-catalyzed carbene chemistry”

23. Baglia, R. A.; Krest, C. M.; Yang, T.; Leeladee, P.; Goldberg, D. P.* *Inorg. Chem.* **2016**, *55*, 10800. “High-Valent Manganese–Oxo Valence Tautomers and the Influence of Lewis/Brönsted Acids on C–H Bond Cleavage”
24. Corcos, A. R.; Pap, J. S.; Yang. T.; Berry, J. F.* *J. Am. Chem. Soc.* **2016**, *138*, 10032. “A Synthetic Oxygen Atom Transfer Photocycle from a Diruthenium Oxyanion Complex”
25. Neu, H. M.; Yang, T.; Baglia, R. A.; Yosca, T. H.; Green, M. T.; Quesne, M. G.; de Visser, S. P.;* Goldberg, D. P.* *J. Am. Chem. Soc.* **2014**, *136*, 13845. “Oxygen-Atom Transfer Reactivity of Axially Ligated Mn(V)−Oxo Complexes: Evidence for Enhanced Electrophilic and Nucleophilic Pathways”
26. Widger, L. R.; Davies, C. G.; Yang, T.; Siegler, M. A.; Troeppner, O.; Jameson, G. N. L.;* Ivanovic-Burmazovic, I.; Goldberg, D. P.* *J. Am. Chem. Soc.* **2014**, *136*, 2699. “Dramatically Accelerated Selective Oxygen-Atom Transfer by a Nonheme Iron(IV)-Oxo Complex: Tuning of the First and Second Coordination Spheres”
27. Widger, L. R.; Jiang, Y.; McQuilken, A. C.; Yang, T.; Siegler, M. A.; Matsumura, H.; Moenne-Loccoz, P.;* Kumar, D.; de Visser, S. P.;* Goldberg, D. P.* *Dalton Trans.* **2014**, *43*, 7522. “Thioether-ligated iron(II) and iron(III)-hydroperoxo/alkylperoxo complexes with an H-bond donor in the second coordination sphere”
28. Neu, H. M.; Quesne, M. G.; Yang, T.; Prokop-Prigge, K. A.; Lancaster, K. M.; Donohoe, J.; DeBeer, S.; de Visser, S. P.;* Goldberg, D. P.* *Chem. Eur. J.* **2014**, *20*, 14584. “Dramatic Influence of an Anionic Donor on the Oxygen-Atom Transfer Reactivity of a Mn^{V}–Oxo Complex”

MANUSCRIPTS

Submitted

1. Wang, Y.-H.; Tseng, Y.-J.; Kumbhar, S. V.; Chen, H.-T.; Yang, T.;* Lu, I.-C.;* Wang, Y.-H.* :Overcoming the Tradeoff Between Reaction Rate and Overpotential in Electrochemical Water Oxidation Using Electronic and Solvent Effects of Dinuclear Cobalt Complex Catalysts”
2. Chuang, Y.-W.; Lu, K.-Y.; Lin, C.-W.; Yang, Y.-C.; Kumbhar, S. V.; Tseng, Y.-J.; Chen, H.-T. Yang, T.*; Lu, I.-C.; Wang, Y.-H. “Exploring Electrochemical C(sp^3)-H Oxidation with Fe(TAML) Complexes: Effect of Ligands on the Reaction Mechanism and Free Energy Relationship”
3. Lin, P.-C.;$^{\perp}$ Yeh, F.-W.;$^{\perp}$ Liu, C.-H.; Wu, G.-C.; Liu, M.-T. Yu, C.-C.;* Yang, T.* “Deciphering the Effect of Aglycones and Glycosidic Linkages on the Divergent Site-selective Fucosylation of LNT and LNnT by FucTa and Bf13FT”

$^{\perp}$**These authors contributed equally**

In preparation

4. Mahato, B.; Yang, T.* “Chemical Insights into Molecular Spin Qubits with Longer Coherence Time by High Throughput Virtual Screening”

ORAL AND WORKSHOP PRESENTATION

Invited

1. "Designing Transition Metal Complexes with Generative AI Models" at: **2024 Chemistry National Meeting**; March 29-31; New Taipei City, Taiwan
2. "What Can Generative Models Do for Quantum Information Processing? A Study Case on the Design of Molecular Qubits with Long Coherence Time" at: **24th East Asian Workshop on Chemical Dynamics**; March 17-21; Taipei, Taiwan
3. "Designing Molecular Transition Metal Complexes Using A Joint Semi-Supervised Variational Autoencoder and Transfer Learning Model" at: **9th Asian Coordination Chemistry Conference**; February 19-22, 2024; Bangkok, Thailand
4. "Inverse Design of Transition Metal Complexes with Desirable Spin States using Generative Neural Networks" at: **International Conference on Molecular Simulation**, National Taiwan University; October 7th, 2023; Taipei, Taiwan
5. "Designing Molecular Transition Metal Complexes Using A Joint Semi-Supervised Variational Autoencoder and Transfer Learning Model" at: Department of Engineering and System Science, National Tsing Hua University; October 4th, 2023; Hsinchu, Taiwan
6. "Inverse Design of Transition Metal Complexes for Catalysis Using Deep Generative Models" at: **Taiwan International Conference on Catalysis**, Department of Chemical Engineering, National Cheng Gung University; June 29th, 2023; Tainan, Taiwan

7. "Designing Transition Metal Complexes for Energy and Storage Applications" at: Department of Chemical Engineering, National Tsing Hua University; April 12th, 2023; Hsinchu, Taiwan
8. "Inverse Design of Ligands for Spin Crossover Materials and of Optoelectronic Materials" at: Department of Chemical Engineering, National Taiwan University; March 15th, 2023; Taipei, Taiwan
9. "Discover Novel OLED and Spin Crossover TM Complexes Using Deep Generative Models" at: Annual Meeting of the Theory Group, National Science and Technology Council; December 17th, 2022; Taipei, Taiwan
10. “Deep Generative Models: A New Method for Molecular Discovery” at T2CoMSA monthly talk; Nov, 24th, 2022; Online
11. “Machine Learning for Molecular Discovery: From Known to Unknown” at Institute for Atomic and Molecular Science; October 6th, 2022; Taipei, Taiwan
12. “AL in Chemistry: from QC Studies to De Novo Design” at: 第四屆化學與材料模擬趨勢暨產業應用論壇, National Taiwan University; September 28th, 2022; Taipei, Taiwan
13. “Developments and Applications of Novel Computer-aided and Deep Learning Methods for Molecule Discovery” at: Department of Chemistry, National Yang Ming Chiao Tung University. April 9th, 2021; Hsin Chu City, Taiwan
14. “Developments and Applications of Novel Computer-aided and Deep Learning Methods for the Discovery of Inorganic Molecular Catalysts and Organic Photodiodes” at: Department of Chemistry, National Tsing Hua University. March 3rd, 2021; Hsin Chu City, Taiwan