

Meng Duan

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Education



B. S., Chemistry
China West Normal University, Sichuan, China 09. 2011 - 06. 2015

Ph. D., Chemistry (advisor: Prof. Yu Lan)
Chongqing University, Chongqing, China 09. 2015 - 06. 2020

Visiting Graduate Student, Chemistry (advisor: Prof. K. N. Houk)
University of California, Los Angeles, USA 10. 2017 - 10. 2019

Experience



Postdoc, Chemistry (advisor: Prof. Peiyuan Yu)
Southern University of Science and Technology, Shenzhen, China 09. 2020 - 10. 2021

Postdoc, Chemistry (advisor: Prof. K. N. Houk)
University of California, Los Angeles, USA 11. 2021 - 01. 2025

Postdoc, Chemistry (advisor: Prof. Benjamin List)
Hokkaido University, Sapporo, Japan 04. 2025 - Present

Research



Quantum mechanics determination of mechanism and origins of stereoselectivity of chiral Brønsted acid-catalyzed asymmetric reactions

Established the origins of regioselectivity of radical attack on substituted aromatics and heterocycles

Determined the binding modes and selectivity of known ligands for cannabinoid receptors CB1 and CB2, and predicted activities of proposed ligands

Publications





1. **Duan, M.**; Shao, Q.; Zhou, Q.; Baran, P. S.; Houk, K. N. Why $\bullet\text{CF}_2\text{H}$ is Nucleophilic But $\bullet\text{CF}_3$ is Electrophilic in Reactions with Heterocycles. *Nat. Commun.* **2024**, *15*, 4630.
2. Wu, Q. H. #; **Duan, M.**#; Chen, Y. #; Yu, P.; Wang, Y. B.; Cheng, J. K.; Xiang, S. H.; Houk, K. N.; Tan, B. Organocatalytic Olefin C–H Functionalization for Enantioselective Synthesis of Atropisomeric 1, 3-Dienes. *Nat. Catal.* **2024**, *7*, 185-194. (co-first author)
3. Chen, Y.#; **Duan, M.**#; Lin, S.; Liu, Y.; Cheng, J. K.; Xiang, S. H.; Yu, P.; Houk, K. N.; Tan, B. Organocatalytic Aromatization-promoted Umpolung Reaction of Imines. *Nat. Chem.* **2024**, *16*, 408-416. (co-first author)
4. **Duan, M.**#; Díaz-Oviedo, C. D.#; Zhou, Y.; Chen, X.; Yu, P.; List, B.; Houk, K. N.; Lan, Y. Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. *Angew. Chem. Int. Ed.* **2022**, *61*, e202113204. (co-first author)
5. Gao, S. #; **Duan, M.**#; Andreola, L. R.; Yu, P.; Wheeler, S. E.; Houk, K. N.; Chen, M. Unusual Enantiodivergence in Chiral Brønsted Acid-Catalyzed Asymmetric Allylation with β -Alkenyl Allylic Boronates. *Angew. Chem. Int. Ed.* **2022**, *61*, e202208908. (co-first author)
6. Yan, Q.#; **Duan, M.**#; Chen, C.; Deng, Z.; Wu, M.; Yu, P.; He, M. L.; Zhu, G.; Houk, K. N.; Sun, J. Organocatalytic Discrimination of Non-directing Aryl and Heteroaryl Groups: Enantioselective Synthesis of Bioactive Indole-containing Triarylmethanes. *Chem. Sci.* **2022**, *13*, 5767-5773. (co-first author)
7. Juliá, F. #; Shao, Q.#; **Duan, M.**#; Plutschack, M. B.; Berger, F.; Mateos, J.; Lu, C.; Xue, X.; Houk, K. N.; Ritter, T. High Site Selectivity in Electrophilic Aromatic Substitutions: Mechanism of C–H Thianthrenation. *J. Am. Chem. Soc.* **2021**, *143*, 16041-16054. (co-first author)
8. Gao, S.#; **Duan, M.**#; Liu, J.; Yu, P.; Houk, K. N.; Chen, M. Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. *Angew. Chem. Int. Ed.* **2021**, *133*, 24298-24308. (co-first author)
9. Li, X.#; **Duan, M.**#; Yu, P.; Houk, K. N.; Sun, J. Organocatalytic Enantioselective Dearomatization of Thiophenes by 1, 10-conjugate Addition of Indole Imine Methides. *Nat. Com.* **2021**, *12*, 4881. (co-first author)
10. Li, X.#; **Duan, M.**#; Deng, Z.#; Shao, Q.; Chen, M.; Zhu, G.; Houk, K. N.; Sun, J. Catalytic Enantioselective Synthesis of Chiral Tetraarylmethanes. *Nat. Catal.* **2020**, *3*, 1010–1019. (co-first author)
11. Gao, S.#; **Duan, M.**#; Shao, Q.; Houk, K. N.; Chen, M. Development of α,α -Disubstituted Crotylboronate Reagents and Stereoselective Crotylation via Brønsted or Lewis Acid Catalysis. *J. Am. Chem. Soc.* **2020**, *142*, 18355-18368. (co-first author)
12. Gao, S.#; **Duan, M.**#; Houk, K. N.; Chen, M. Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with α -Vinyl Allylboron Reagents. *Angew. Chem. Int. Ed.* **2020**, *59*, 10540-10548. (co-first author)
13. Zhang, R.#; Guo, W.#; **Duan, M.**#; Houk, K. N.; Sun, J. Asymmetric Desymmetrization of Oxetanes for the Synthesis of Chiral Tetrahydrothiophenes and Tetrahydroselenophenes. *Angew. Chem. Int. Ed.* **2019**, *58*, 18055–18060. (co-first author)



14. **Duan, M.**[#]; Zhu, L.[#]; Qi, X.; Yu, Z.; Li, Y.; Bai, R.; Lan, Y. From Mechanistic Study to Chiral Catalyst Optimization: Theoretical Insight into Binaphthophosphine-Catalyzed Asymmetric Intramolecular [3 + 2] Cycloaddition. *Sci. Rep.* **2017**, *7*, 1–13. (co-first author)
15. Adak, S.; Ye, N.; Calderone, L. A.; **Duan, M.**; Lubeck, W.; Schäfer, R. J. B.; Lukowski, A. L.; Houk, K. N.; Pandelia, M.; Drennan, C. L.; Moore, B. S. A Single Diiron Enzyme Catalyses the Oxidative Rearrangement of Tryptophan to Indole Nitrile. *Nat. Chem.* **2024**, 1–10.
16. Kang, W. J.; Li, B.; **Duan, M.**; Pan, G.; Sun, W.; Ding, A.; Zhang, Y.; Houk, K. N.; Guo, H. Discovery of a Thioxanthone–TfOH Complex as a Photoredox Catalyst for Hydrogenation of Alkenes Using p-Xylene as both Electron and Hydrogen Sources. *Angew. Chem. Int. Ed.* **2022**, *61*, e202211562.
17. Liu, F.; Ma, S.; Lu, Z.; Nangia, A.; **Duan, M.**; Yu, Y.; Xu, G.; Mei, Y.; Bietti, M.; Houk, K. N. Hydrogen Abstraction by Alkoxy Radicals: Computational Studies of Thermodynamic and Polarity Effects on Reactivities and Selectivities. *J. Am. Chem. Soc.* **2022**, *144*, 6802–6812.
18. Martin, T.; Galeotti, M.; Salamone, M.; Liu, F.; Yu, Y.; **Duan, M.**; Houk, K. N.; Bietti, M. Deciphering Reactivity and Selectivity Patterns in Aliphatic C–H Bond Oxygenation of Cyclopentane and Cyclohexane Derivatives. *J. Org. Chem.* **2021**, *86*, 9925–9937.
19. Zhu, L.; Ye, J. H.; **Duan, M.**; Qi, X.; Yu, D. G.; Bai, R.; Lan, Y. The Mechanism of Copper-Catalyzed Oxytrifluoromethylation of Allylamines with CO₂: A Computational Study. *Org. Chem. Front.* **2018**, *5*, 633–639.
20. Yu, Z.; Jin, Z.; **Duan, M.**; Bai, R.; Lu, Y.; Lan, Y. Toward a Predictive Understanding of Phosphine-Catalyzed [3 + 2] Annulation of Allenolates with Acrylate or Imine. *J. Org. Chem.* **2018**, *83*, 9729–9740.
21. Xu, D.; Qi, X.; **Duan, M.**; Yu, Z.; Zhu, L.; Shan, C.; Yue, X.; Bai, R.; Lan, Y. Thiolate–Palladium(IV) or Sulfonium–Palladate(0)? A Theoretical Study on the Mechanism of Palladium-Catalyzed C–S Bond Formation Reactions. *Org. Chem. Front.* **2017**, *4*, 943–950.
22. Yu, J.; **Duan, M.**; Wu, W.; Qi, X.; Xue, P.; Lan, Y.; Dong, X. Q.; Zhang, X. Readily Accessible and Highly Efficient Ferrocene-Based Amino-Phosphine-Alcohol (f-Amphol) Ligands for Iridium-Catalyzed Asymmetric Hydrogenation of Simple Ketones. *Chem. Eur. J.* **2017**, *23*, 970–975.
23. Zhu, L.; Qi, X.; Li, Y.; **Duan, M.**; Zou, L.; Bai, R.; Lan, Y. Ir(III)/Ir(V) or Ir(I)/Ir(III) Catalytic Cycle? Steric-Effect-Controlled Mechanism for the Para-C–H Borylation of Arenes. *Organometallics* **2017**, *36*, 2107–2115.
24. Wu, W.; Liu, S.; **Duan, M.**; Tan, X.; Chen, C.; Xie, Y.; Lan, Y.; Dong, X. Q.; Zhang, X. Iridium Catalysts with f-Amphox Ligands: Asymmetric Hydrogenation of Simple Ketones. *Org. Lett.* **2016**, *18*, 2938–2941.