

Min GAO
Associate Professor (Tenure track)
Junior Principal Investigator

Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University
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Basic Information

Nationality: Chinese

Research keywords: computational catalysis, solid-state material, metal cluster, organic catalyst

Languages: Chinese (native), Japanese (fluent, JLPT N1), English (fluent)

Hobbies: Outdoor events, running, baseball practice, hiking

Research Experience

Associate Professor 2022.8 ~ Now: Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University, Japan

Assistant Professor 2018.7- 2022.7: Catalysis Theory Research Division, Institute for Catalysis (ICAT), Hokkaido University, Japan

Assistant Professor 2016.1- 2018.6: Quantum Chemistry Lab, Department of Chemistry, Faculty of Science, Hokkaido University, Japan

Postdoc Fellow 2012.10-2015.12: Quantum Chemistry Lab, Department of Chemistry, Faculty of Science, Hokkaido University, Japan

Education

Ph.D., Science, 2009.10-2012.09 Hokkaido University, Japan.

Supervisor: Prof. Taketsugu Tetsuya

M.S., Chemistry, 2007.09-2009.06 Tianjin University, China

Supervisor: Prof. Taketsugu Tetsuya and Assist. Prof. Maeda Satoshi (Prof. Maeda Satoshi)

B.S., Chemistry, 2003.09-2007.06 Nanachang Hangkong University, China

Awards

1. *The 3rd Young Researcher Award of Japan Society of Theoretical Chemistry* with the title

of “Mechanistic understanding and design guidelines for heterogeneous catalysis based on systematic structural calculations” Apr. 2022 (第3回理論化学会奨励賞 「系統的な構造計算に基づく不均一系触媒の機構理解と設計指針の構築」)

2. *Outstanding Lecture Award in Molecular Science* with title of “Large active area of h-BN Monolayer induced by carbon doping” at the 10th Annual Meeting of Japan Society for Molecular Science Kobe, Japan, Sept. 13th-16th, 2016 (第10回分子科学討論会 分子科学優秀講演賞, 神戸, 2016年9月13日-16日)
3. *Best Poster Award* with the title of “Automated reaction path search for the mechanism of C(sp³)-H activation catalyzed by Si-supported monophosphine-Ir(III)” at the 15th International Congress of Quantum Chemistry”, Beijing, China. Jun. 8th-13th, 2015
4. *Best Poster Award* with the title of “Exploring reaction pathway of H₂ dissociation on Au_n (n = 1–10) clusters by automated reaction path search methods” at the 16th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, Sapporo, Japan. Aug. 4th-9th, 2013
5. *Fujitsu Poster Award* with the title of “Catalytic activity of gold clusters on the inert h-BN surface” at the Seventh Congress of the International Society for Theoretical Chemical Physics, Tokyo, Japan. Sept. 2nd-8th, 2011

Research Projects

1. ○Min Gao
2017.04—2018.04 Grants-in-Aid for Scientific Research Young Researchers B (Issue Number: 17K1442907) “若手研究B : Large range functionalization of h-BN monolayer by carbon doping”
2. ○Min Gao
2020.04—2023.04 Grant-in-Aid for Scientific Research, Fundamental Research C (Issue Number: 20K05217) “基盤研究C : 金属ナノ粒子の触媒活性見たい目判別に向けた遷移状態の情報化学的研究”
3. ○Min Gao
2018.07 ~2019.04 Hokkaido University Young Researcher Research Acceleration Programme” 創成若手研究加速支援事業 : CH₄解離反応に対する金属クラスター触媒活性の理論予測”
4. ○Min Gao

2021.10 Hokkaido University Cross-Departmental Symposium Research Grant” 部局横断型若手研究助成：排ガス浄化に必須となるアルカリ被毒耐性を備えた次世代脱硝触媒の理論解析”

Invited Talks

1. M. Gao, "Theoretical investigations on the Activation of Small Gas Molecules on free and surface supported metal clusters"
International Symposium on Air Pollution Control Chemistry, Shanghai, online Conference, Nov. 18th, 2021
2. M. Gao, "Theoretical simulations of heterogeneous catalysis"
12th CSE Autumn School & the 9th ALP International Symposium, online Conference, Hokkaido University, Oct. 13th-14th, 2021
3. M. Gao, "Theoretical studies on the catalytic activity of metal clusters based on systematic structural calculations."
The 128th CATSJ Meeting, Kyoto University (online), Sept. 15th-17th, 2021
「系統的な構造計算に基づく金属クラスターの触媒活性に関する理論研究」
第128回触媒討論会, 京都大学, オンライン開催, 2021年9月15-17日
4. M. Gao, "Tunable catalytic performance of metal clusters by morphology control"
International Conference on Advanced Catalysts for Energy and Environmental Applications, Shanghai, Online Conference, Apr. 12th-13th, 2021.
5. M. Gao, "Theoretical investigation on catalytic activity of metal clusters"
The International Symposium on Advanced Catalyst Design and Molecular Catalysis, Xi'an, China (Online Conference), Aug. 31st-Sept. 4th, 2020
6. M. Gao, "Computational Catalysis: Theory, Models and Applications"
The 59th Aurora seminar, Hokkaido, Jul. 21st, 2019 (高敏「理論化学の視点からの触媒 (Computational Catalysis: Theory, Models and Applications)」第59回オーロラセミナー, 北海道, 2019年7月21日)
7. M. Gao "Theoretical study of the geometry and size effect on the catalytic activity of gold clusters"
International Congress on Pure & Applied Chemistry (ICPAC) 2018 Sokhalay Angkor Resort & Spa, Siem Reap, Cambodia, Mar. 6th, 2018.
8. M. Gao "Reactivity of Gold Clusters in the Regime of Structural Fluxionality"
The 21st International Annual Symposium on Computational Science and Engineering, Thailand Science Park, Pathum Thani, Thailand, Aug. 4th, 2017.
9. M. Gao "A theoretical design of catalyst based on h-BN surface"
Thai-Japan Symposium in Chemistry, Nov. 15th, 2016.
10. **(Outreach activities)** M. Gao "My Research & life in Hokkaido University (Importance of

Communication)” Career Seminar for international students in Science Dec. 2017
2017年12月 北海道大学 理系大学院留学生のための就職研究セミナー

Committee Memberships

1. May 2016~ April 2018: Committee member of Hokkaido Branch of the Catalysis Society of Japan
2. May 2018~ April 2020: Committee member of Public Relations, Catalysis Society of Japan; Vice-Committee member of Hokkaido Branch HP. (触媒学会広報副委員北海道支部HP副委員)
3. May 2020 ~ Now member of PR Committee; HP committee of Hokkaido Branch of Catalysis Society of Japan (触媒学会 広報委員、北海道支部HP委員)
4. April 2022 ~ Now Committee member of the Catalysis Society's 'WG on the Future of Catalysis' (触媒学会「触媒の未来を考えるWG」委員)

Helped Organized Conference

1. 2019/5/27-29 Executive Committee of The 22nd Annual Meeting of Japan Society of Theoretical Chemistry (第22回理論化学討論会 実行委員会)
2. 2019/10/31 Executive Committee of Hokkaido University cross-departmental symposium (北海道大学部局横断シンポジウム 実行委員会)
3. 2019/09/28 Executive Committee of Hokkaido University cross-departmental symposium (北海道大学部局横断シンポジウム 実行委員会)
4. 2021/09/28-21 Executive Committee of The 15th Annual Meeting of Japan Society for Molecular Science (第15回分子科学討論会 実行委員会)