Curriculum Vitae of Ming Lei

ADDRESS

Ming Lei Ph.D
Professor
State Key Laboratory of Chemical Resource Engineering
Institute of Computational Chemistry, College of Chemistry
PO Box 105
Beijing University of Chemical Technology
BeiSanHuan East Road 15th
Beijing 100029
P.R. China
Tel: +86-10-64446598(O)
Email: leim@mail.buct.edu.cn
http://minglab.cn

PERSONAL DATA

Male; Born: 1972, Nov.; Hunan Prov., P. R. China; Married

EMPLOYMENT HISTORY

Beijing University of Chemical Technology (BUCT):

Apr., 2020 – present	Professor in College of Chemistry of BUCT
Jan., 2015 – Mar., 2020	Professor in College of Science of BUCT
Nov., 2005 – Dec., 2014	Associate Professor in College of Science of BUCT
July, 2011 – July, 2012	Deputy Dean of Graduate School of BUCT
Nov., 2008 – July, 2011	Deputy Director of International Exchanges&Cooperation Department of BUCT
July, 2000 – Oct., 2005	Lecturer in Department of Applied Chemistry of BUCT

EDUCATION

July, 2014 – Sept., 2014	Visiting Professor in Fukui Institute of Fundamental Chemistry in Kyoto University (Kyoto, Japan).
July, 2008 – Sept., 2008	Visiting Professor in Cherry L. Emerson Center in Emory University (Atlanta, GA, USA).
Jan., 2002 – Jan., 2005	Postdoctoral Research Associate in Biophysical and Computational Chemistry in Clark University (Worcester, MA, USA), Supervisor: Prof. Shuanghong Huo
Sept., 1997 – June, 2000	Ph. D in Applied Chemistry (Computational Chemistry) in Beijing University of Chemical Technology (Beijing, China), Advisor: Prof. Wenlin Feng
Sept., 1994 – June, 1997	M.S. in Applied Quantum Chemistry (Computational Chemistry) in Beijing Normal University (Beijing, China), Advisor: Prof. Wenlin Feng

Sept., 1990 – June, 1994 B.S. in Chemistry in Hunan Normal University (Changsha City, Hunan Province)

PROFESSIONAL RESEARCH

Ming Lei has published 172 peer-review papers with H-index of 26.

Theoretical Studies on Organometallic Catalysis

Due to applications in industrial and synthetic processes of catalytic transition-metal reactions, ab initio molecular orbital (MO) and density functional theory (DFT) methods are used to study a series of transition-metal-catalyzed chemical reactions. Here, we focus on reaction mechanisms of transition-metal chiral catalysis involving various classes of elementary reactions such as substitution, migratory insertion, hydrogen transfer, oxidative addition/reductive elimination, metathesis, and nucleophilic addition.

By means of theoretical and computational chemistry, we investigated reaction mechanisms of small molecule activation, C-H bond activation and asymmetric reaction catalyzed by organometallic complexes systematically, including the activation of dihydrogen, nitrogen, carbon dioxide and olefins et al. Some fundamental reactions such as substitution, migration and insertion, hydrogen transfer, oxidative addition/reductive elimination, metathesis and nucleophilic addition were discussed. The mechanisms of organometallic catalytic reactions were summarized to unveil the nature of reaction activity and selectivities. The factors like solvent effect on organometallic catalysis were considered. Meanwhile, the three-dimensional quantitative structure performance relationship (3D-QSPR) model was established, which could promote the design and discovery of new skeleton transition metal catalyst with high activity and enantioselectivity based on the reaction mechanism (this is supported by NSFC grant Nos: 21672018, 2161101308, 21373023, 21072018).

Theoretical Studies on Catalysis on Surfaces

The first-principles theory and DFT method are used to study the heterogeneous catalysis on surfaces. Here we focus on reaction mechanisms of catalysis on surfaces involving metal oxides related to small molecules activation in sustainable energy field, to unveil the nature of heterogeneous catalysis and build relationship between structures of surfaces and their catalytic activities (this is supported by NSFC grant No: 22073005).

Computational Biophysical Chemistry

The three-dimensional structure and dynamics are closely related with the function of biomolecules. By means of QM/MM, molecular dynamic simulation, docking and 3D-QSAR methods, the relationship between the dynamics and the function of the molecule and biocatalysis mechanism at atomic level were investigated, which be very useful to design new drugs on biomolecular targets. Quantum mechanics with molecular mechanics (QM/MM) method is used to investigate biomolecular catalytic mechanisms (this is supported by NSFC grant No: 20703003).

Software Development (J project)

J project aims on the development of a GUI software to construct molecules, display the model, investigate reaction mechanism, perform data mining, build QSAR relationship. This will be used to develop new catalysts based on reaction mechanisms. In addition, some education functions will also be developed such as point group conception.

PROFESSIONAL SKILLS

Quantum chemistry tools: Gaussian, QChem, Terachem, and so on,
Molecular simulation tools: VASP, Materials Studio, Amber, Charmm, NAMD, and so on,
Drug discovery tools: SYBYL, MOE, Schrodinger etc.
Programming tools: Fortran, C, and Python etc.
Linux administration and Linux script languages like Bash/C shell languages.

PROFESSIONAL ASSOCIATION

Chinese Chemical Society (CCS), America Chemical Society (ACS), Asia-Pacific Association of Theoretical & Computational Chemists (APATCC)

AWARDS

Nov, 2017	Distinguished Young Teacher Award in BUCT
May, 2009	Second-class Beijing High Education Teaching Award of 2008,
Aug., 2008	Beijing Outstanding Youth Scientist (Winner of Beijing Nova Fund)
Apr., 2008	Outstanding Young Teacher Award in BUCT,
Jan., 2000	BUCT-BASF Outstanding Ph.D Student Award.

RESEARCH SUPPORT

PGA project sponsored by SINOPEC Beijing Research Institute of Chemical Industry (BRICI), PI: Ming Lei, 2022-2023
National Natural Science Foundation of China (NSFC, Grant No. 22073005), PI: Ming Lei, 2021-2024
PBST project sponsored by SINOPEC Beijing Research Institute of Chemical Industry (BRICI), PI: Ming Lei, 2021-2022
National Natural Science Foundation of China (NSFC, Grant No. 21672018), PI: Ming Lei, 2017-2020
The Joint Research Fund of National Natural Science Foundation of China (NSFC) and Royal Society of UK (RS) (NSFC-RS Grant No. 2161101308), PI: Ming Lei, 2017-2019
Fundamental Research Funds for the Central Universities, MOE (FRFCU Grant No. PYCC1708), PI: Ming Lei, 2017
The Special Program for Applied Research on Super Computation of the NSFC-Guangdong Joint Fund (the second phase) PI: Ming Lei, 2015-2017
Beijing Municipal Natural Science Foundation (BJNSF, Grant No. 2162029), PI: Ming Lei, 2016-2018
BUCT Fund for Disciplines Construction and Development (Grant No. XK1527), PI: Ming Lei, 2015-2016
National Natural Science Foundation of China (NSFC, Grant No. 21373023), PI: Ming Lei, 2014-2017
Open Research Fund of State Key Laboratory of Natural and Biomimetic Drugs in Peking University. (ORF of SKLNBD, Grant No. K20120202), PI: Ming Lei, 2012-2013
National Natural Science Foundation of China (NSFC, Grant No. 21072018), PI: Ming Lei, 2011-2013
Fundamental Research Funds for the Central Universities, MOE (FRFCU Grant No. ZZ1020), PI: Ming Lei, 2010-2011

Open Research Fund of State Key Laboratory of Natural and Biomimetic Drugs in Peking University. (ORF of SKLNBD, Grant No. K20100103), PI: Ming Lei, 2010
National Natural Science Foundation of China (NSFC, Grant No. 20703003), PI: Ming Lei, 2008-2010
Scientific Research Foundation for the Returned Overseas Chinese Scholars (SRF for ROCS, SEM), PI: Ming Lei, 2006-2008
Drug Discovery of ANT using VHS sponsored by NHWa Corp., PI: Ming Lei, 2006-2008
Beijing Nova Fund (Grant No. 2005B17), PI: Ming Lei, 2005-2008
Young Teachers' Foundation of Beijing University of Chemical Technology, PI: Ming Lei, 2000-2001

COURSES TAUGHT

Structure Chemistry (Undergraduate Students), 2015-present (Fall)
Advanced Physcial Chemistry (Graudate Students), 2023-present (Fall)
Computational Catalysis (Graduate Students), 2019-present (Spring)

REVIEW SERVICE TO PROFESSIONAL JOURNALS

Nature Catalysis
Nature Communications
Journal of the American Chemical Society
ACS Catalysis
ACS Applied Materials & Interfaces
Crystal Growth & Design
Inorganic Chemistry
The Journal of Organic Chemistry
The Journal of Physical Chemistry
Organometallics
Langmuir
Industrial & Engineering Chemistry Research
iScience
Angewandte Chemie-International Edition
ChemCatChem
Journal of Materials Chemistry A
Physical Chemistry Chemical Physics
Organic & Biomolecular Chemistry
Chemical Science
Dalton Transaction
Catalysis Science and Technology
New Journal of Chemistry
Green Chemistry
RSC Advance
Asian Journal of Organic Chemistry
European Journal of Inorganic Chemistry
Catalysis Letters
Catalysis Communications

Computational & Theoretical Chemistry
Journal of Organometallic Chemistry
Journal of Molecular Catalysis B: Enzymatic
Journal of Photochemistry and Photobiology A: Chemistry
Journal of Physical Organic Chemistry
Chemical Biology & Drug Design
Journal of Molecular Graphics and Modelling
Archives of Pharmacal Research
Computer Methods and Programs in Biomedicine
Genomics, Proteomics & Bioinformatics
Molecular Simulation
Journal of Experimental Nanoscience
Journal of Control Science and Engineering
Journal of Functional Biomaterials
Synthetic Metals
Applied Biochemistry and Biotechnology
Theoretical Chemistry Accounts
Science China Chemistry
Acta Physico-Chimica Sinica
Chemical Journal of Chinese Universities
Frontiers of Chemical Science and Engineering
Scientia Sinica Chimica
Sciencepaper Online
Chinese Journal of Structural Chemistry
CIESC Journal (Chemical Industry and Engineering Society of china)

GROUP MEMBERS:

GRADUATE STUDENTS

Xiaofan Shi	Ph.D Student (2022-present)	
Zhewei Li	Ph.D Student (2021-present)	
Soomro Irfan Ali	Ph.D Student (2021-present)	
Haohao Wang	Ph.D Student (2019-present)	
Yulan Dai	Ph.D 2023 (2019-2023)	
Qaim Ali	Ph.D Student (2018-present)	
Yangqiu Liu	Ph.D Student (2018-present)	
Wei Zhang	Ph.D 2021 (2016-2021)	Associate Professor in Shihezi University
Xingyu Chen	Ph.D 2022 (2015-2022)	Researcher in AsymChem
Longfei Li	Ph.D 2018 (2015-2018)	Associate Professor in Hebei University
Hui Li	Ph.D 2017 (2014-2017)	Lecturer in North Minzu University
Xuelu Ma	Ph.D 2015 (2010-2015)	Associate Professor in China University of Mining & Technology, Beijing
Mawia H. Elsaim	Ph.D 2012 (2009-2012)	Lecturer in Sudan

Shilong Li	MA student (2023-present)	
Wei Li	MA student (2023-present)	
Hongyun Cui	MA student (2023-present)	
Yin Gai	MA student (2022-present)	
Qiong Peng	MA student (2022-present)	
Shuo Zhang	MA student (2022-present)	
Yin Gai	MA student (2021-present)	
Yunfan Yue	MA student (2021-present)	
Jirui Du	MA student (2021-present)	
Hexiang Qi	MA student (2021-present)	
Tian Ma	MA student (2021-present) with Assoc. Prof. Zuoyin Yang	
Dengyu Jin	MA 2023 (2020-2023)	Northern Huian Chem. Industry Corp.
Caiwei Yue	MA 2023 (2020-2023)	Darbond Technology Co. Ltd
Jing Wen	MA 2023 (2020-2023)	
Ruixue Zhang	MA 2023 (2020-2023)	Ph.D student in China University of Petroleum (Beijing)
Rui Wang	MA 2022 (2019-2022)	China Construction Bank Taian
Chong Liu	MA 2022 (2019-2022)	Ph.D student in China University of Petroleum (East China)
Yaqi Zhao	MA 2022 (2019-2022) with Prof. Min Pu	Ph.D student in Peking University
Fuxing Shi	MA 2022 (2019-2022) with Prof. Li Liu and Prof. Xiaolin Li	Ph.D student in Max-Planck-Institut für Kohlenforschung
Yuting Tao	MA 2021 (2018-2021) with Assoc. Prof. Zuoyin Yang	Ph.D student in Beijing Institute of Technology
Xiaodi Zhang	MA 2021 (2018-2021)	Researcher in Rianlon Corp.
Lin Zhang	MA 2021 (2018-2021)	Ph.D student in Xiamen University
Qianyue Wang	MA 2020 (2017-2020)	SINOPEC Beijing Institute of Chemical Industry
Ruiqing Ding	MA 2020 (2017-2020)	Qingdao Institute of Bioenergy and Bioprocess Tech., CAS
Chenguang Luo	MA 2020 (2017-2020)	BOE Company
Xin Yue	MA 2019 (2016-2019)	XtalPi Company
Pengjie Li	MA 2019 (2016-2019)	Postdoc of Huazhong University of Science and Technology
Yiwei Zhang	MA 2017 (2014-2017)	Ph.D student of Huazhong University of Science and Technology
Yanxia Xi	MA 2017 (2014-2017)	
Xinli Duan	MA 2016 (2013-2016)	National Institute of Measurement of China
Zhidong Wang	MA 2016 (2012-2016)	
Yuhui Pan	MA 2015 (2012-2015)	
Min Zhao	MA 2014 (2011-2014)	
Min Wang	MA 2014 (2011-2014)	
Lijun Zhao	MA 2013 (2010-2013)	Sale staff in company
Ran Feng	MA 2013 (2010-2013)	Technical staff in company
Xiaojie Du	MA 2013 (2010-2013)	Technical staff in company
Qian Shen	MA 2012 (2010-2012)	Technical staff in company
Tianhu Yuan	MA 2012 (2009-2012)	Officer in Chongqing Customs

Xiaojia Guo	MA 2012 (2009-2012)	Staff in company
Wenchao Zhang	MA 2011 (2008-2011)	Technical staff in company
Zhuo Chen	MA 2010 (2006-2010)	Technical staff in BOEOT
Baohua Zhang	MA 2010 (2006-2010)	Technical support Staff in SCCAS
Ang Xiao	MA 2010 (2006-2010)	Technical staff in BOEOT
Yue Chen	MA 2009 (2006-2009)	Postdoc in Kyoto University
Houfang Wang	MA 2008 (2005-2008)	Staff in Tri-ibiotech Corp.

UNDERGRADUATE RESEARCH STUDENTS

Ziqiang Chen	B.S. 2023
Ao Sheng	B.S. 2023
Weiqing Du	B.S. 2023
Yongyong Chen	B.S. 2023
Jingling Du	B.S. 2023
Junhong Qiu	B.S. 2023
Chenyu Wu	B.S. 2022
Longfei Chang	B.S. 2022
Jiuyang Wu	B.S. 2022
Xiaofan Shi	B.S. 2022
Yin Zhou	B.S. 2022
Chenxi Sheng	B.S. 2022
Shilong Li	B.S. 2022
Haoran Yang	B.S. 2022
Wenxin Li	B.S. 2021
Liwei Ye	B.S. 2021
Shuoran Yang	B.S. 2021
Xinpeng Yuan	B.S. 2021
Peixin Liu	B.S. 2021
Sifan Hu	B.S. 2021
Hexiang Qi	B.S. 2021
Zhuo Quan	B.S. 2021
Anqi Liu	B.S. 2021
Yinxing Zou	B.S. 2021
Zhewei Li	B.S. 2021
Ling Zhu	B.S. 2020
Xiaochuan Ren	B.S. 2020
Yunfeng Tu	B.S. 2020
Xiaoliang Liu	B.S. 2020
Fengze Han	B.S. 2020
Zhetang Chen	B.S. 2019
Hao Xin	B.S. 2019
Zhipeng Wang	B.S. 2019
Ding Peng	B.S. 2019
Yangqiu Liu	B.S. 2018
Xiaodi Zhang	B.S. 2018
Zenghui Duan	B.S. 2018
Junlin Qiu	B.S. 2018
Guohang Huo	B.S. 2018
Guihong Li	B.S. 2018
Quan Yuan	B.S. 2018
Tong Sheng	B.S. 2017

Zheng Zuo	B.S. 2017	
Xinyu Gong	B.S. 2017	
Tong Zhou	B.S. 2017	
Hongyin Zhou	B.S. 2017	
Xin Qu	B.S. 2017	
Xinxin Fang	B.S. 2017	
Yue Mo	B.S. 2015	
Zihao Fan	B.S. 2015	
Jiyang Zhu	B.S. 2015	
Fulong Liu	B.S. 2015	
Yiwei Zhang	B.S. 2014	
Mo Zhang	B. S.2014	
Yan Hu	B.S. 2010	Ph.D Stud. in Univ. of Iowa in USA
Wenzheng Xie	B.S. 2010	Staff in Beijing Yuhua Coorp
Weiwei Xie	B.S. 2009	Grad. Stud. in Instit. of Chem., CAS
Lingzhou Zhao	B.S. 2009	Grad. Stud. in Beijing Normal Univ.
Tianhu Yuan	B.S. 2009	Grad. Stud. at Beijing Univ. of Chem. Tech.
Chunli Zhao	B.S. 2009	
Yuanfu Yu	B.S. 2008	Pharmacy in Tianjing
Yunhan Li	B.S. 2008	
Zehan Hu	B.S. 2008	(2006-2008) Tenure-track Associate Professor in Shanghai Jiaotong University
Hongbo Zhang	B.S. 2007	Grad. Stud. in Beijing Univ. of Chem. Tech.
Hongjun Xie	B.S. 2006	
Ruqiang Liu	B.S. 2006	Grad. Stud. in Capital Normal Univ.
Yue Chen	B.S. 2006	Postdoc in Kyoto University

PUBLICATIONS:

172. Yunfan Yue, Tian Ma, Hexiang Qi, Yaqi Zhao, Xiaofan Shi, Yanhui Tang, Min Pu, **Ming Lei*** (2023) "The Theoretical Design of Manganese Catalysts with Si-N-Si-C-Si-C Six-membered Ring Core-based Bowl-shaped Quadridentate Ligand for the Hydrogenation of C=O/C=N Bonds." Phys. Chem. Chem. Phys., DOI:10.1039/D3CP03217E
171. Xianglin Luo‡, Zhewei Li‡, Yuzhen Zheng, Yueping Lin, Huanfeng Jiang, Lukas J. Gooßen*, **Ming Lei***, Liangbin Huang* (2023) "Ligand-Enabled ortho-Arylation of (hetero)Aromatic Acids with 2,6-Disubstituted Aryl Halides." ACS Catal., 13(18): 12104-12113 (‡ Co-first author)
170. Haohao Wang, Caiwei Yue, Jirui Du, Min Pu, and **Ming Lei*** (2023) "First Principles Study on the Mechanism of Nitrobenzene Hydrogenation by a Ni1/CeO2-x(111) Single-Atom Catalyst." J. Phys. Chem. C, 127(34): 16880-16890
169. Ziqiang Chen, Hexiang Qi, Haohao Wang, Caiwei Yue, Yangqiu Liu, Zuoyin Yang*, Min Pu, **Ming Lei*** (2023) "The Rational Design of High-performance Carbon-based Electrocatalysts for ORR Using Machine Learning." Phys. Chem. Chem. Phys., 25(28): 18983-18989
168. Zhenli Luo‡, Zhewei Li‡, Haoqiang Zhao‡, Ji Yang, Lijin Xu*, **Ming Lei***, Qinghua Fan, Patrick J. Walsh* (2023) "Borane-Catalyzed Tandem Cyclization/Hydrosilylation Towards Enantio- and Diastereoselective Construction of trans-2,3-Disubstituted-1,2,3,4-Tetrahydroquinoxalines." Angew. Chem. Int. Ed., 62(32): e202305449 (‡ equal contribution)
167. Yulan Dai, Zhewei Li, Min Pu, **Ming Lei*** (2023) "Understanding the Mechanism and Selectivity of 1,1-Diborylalkanes from Alkenes Catalyzed by Zirconium Complex." Inorg. Chem., 62(27): 10854-10864
166. Fang Yu*, Tian Ma, Wenbin Liang, **Ming Lei*** (2023) " A DFT Mechanistic Study on the

N-acyloxyamine-initiated Controlled Degradation of Polypropylene.” J. Applied Polymer Sci., 140(33): e54295

165. Dengyu Jin, Jinjiang Xu*, Haobin Zhang, **Ming Lei***, Jie Sun* (2023) “Comparative Study of Experiments and Calculations on the Guest Molecules’ Escaping Mechanism of CL-20-Based Host-Guest Energetic Materials.” J. Phys. Chem. C, 127(24): 11641-11651
164. Jing Wen, Zhewei Li, Yanhui Tang, Min Pu*, **Ming Lei*** (2023) “Mechanistic Insight of Amides Formation from Aryl Epoxides and Amines Catalyzed by Ruthenium Pincer Complexes: A DFT Study.” Dalton Trans., 52(24): 8449-8455
163. Bin Wang, Chunying Rong*, **Ming Lei***, Shubin Liu*, Frank De Proft* (2023) “Mechanistic Study and Conceptual Chemical Reactivity Analysis of Hydroboration of Carbon Dioxide Catalyzed by a Manganese(I)-PNP-Pincer Complex.” Inorg. Chem., 62(19): 7366-7375
162. Qaim Ali, Zhewei Li, Lin Zhang, Chenguang Luo, Min Pu, **Ming Lei*** (2023) “DFT Mechanistic Investigation on Manganese Pincer Complex Catalyzed Cross-coupling of Methanol with Benzyl Alcohol to Afford Methyl Benzoate.” Chem. Eur. J., 29(35): e202300565
161. Yangqiu Liu, Hexiang Qi, **Ming Lei*** (2023) “Improved Elastic Image Pair Method for Finding Transition States.” J. Chem. Theory Comput., 19(8): 2410-2417
160. Peihuan Zhang, Yue Zhu, Zhewei Li, Luocong Wang, Caiwei Yue, **Ming Lei***, Min Pu* (2023) “Theoretical Study on Photothermal Properties of Azobenzene Sulfonate/Magnesium-Aluminum Hydroxide Composite Dye.” ACS Omega, 8(12): 11596-11606
159. Kai Jiang ‡, Haohao Wang ‡, Yi Xie, Huanfeng Jiang, **Ming Lei***, Biaolin Yin* (2023) “Remote-Group-Assisted Facile Oxidative Arylation of Furans and Pyrroles.” ACS Catal., 13(6): 3520-3531 (‡ equal contribution)
158. Xudong Sun‡, Xiaotong Yu‡, Yaqi Zhao‡, Lei Xing, Luxin Na, Zhuo Chen, Zhangping Xiao, Hong Dai, Jing Yu, Sijie Long, Quanxin Wang, Xiaofan Shi, Zhu Guan, **Ming Lei***, Zhenjun Yang* (2023) “Cyclic Diguanylate Analogues: Facile Synthesis, STING Binding Mode and Anti-tumor Immunity Delivered by Cytidinyl/cationic Lipid.” Eur. J. Med. Chem., 247: 115053 (‡ equal contribution)
157. Xuelu Ma*, Meng Li, **Ming Lei*** (2023) “Trinuclear Transition Metal Complexes in Catalytic Reactions.” Acta. Chim. Sin., 81(1): 84-99 (马雪璐*, 李蒙, 雷鸣* (2023) “三核过渡金属配合物在催化反应中的研究进展” 化学学报 81(1): 84-99)
156. Hexiang Qi, Zhipeng Wang, Ding Peng, Fengze Han, Yangqiu Liu, Min Pu, Zuoyin Yang, Yaping Li, Sai An, **Ming Lei*** (2022) “Identification of Point Group of Molecules.” Univ. Chem., 37(12): 2112038 (祁鹤翔, 王智鹏, 彭鼎, 韩丰泽, 刘阳秋, 蒲敏, 杨作银, 李亚平, 安赛, 雷鸣* (2022) “分子点群的判别” 大学化学 37(12): 2112038)
155. Qaim Ali, Yongyong Chen, Ruixue Zhang, Zhewei Li, Yanhui Tang, Min Pu, **Ming Lei*** (2022) “The Origin of Stereoselectivity in the Hydrogenation of Oximes Catalyzed by Iridium Complexes: A DFT Mechanistic Study.” Molecules, 27(23): 8349
154. Yulan Dai, Binfang Yuan, Zhewei Li, Lin Zhang, Longfei Li, Min Pu, **Ming Lei*** (2022) “Density Functional Theory Study on the H2-Acceptorless Dehydrogenative Boration of Alkenes Catalyzed by a Zirconium Complex.” J. Org. Chem., 87(24): 16632-16643
153. Baiyao Zhu‡, Zhewei Li‡, Fulin Chen‡, Wenfang Xiong, Xiaobin Tan, **Ming Lei***, Wanqing Wu, Huanfeng Jiang* (2022) “Palladium-Catalyzed Oxidative Heck Reaction of Non-activated Alkenes Directed by Fluorinated Alcohol.” Chem. Commun., 58(91): 12688-12691 (‡ equal contribution)
152. Lulu Zhang, Caiwei Yue, Lin Zhang, Peihuan Zhang, Luocong Wang, **Ming Lei***, Min Pu* (2022) “A DFT Study on the Isomerization Mechanism of Azobenzene Derivatives on Silicon Substrate.” New J. Chem., 46(45): 21553-21559
151. Caiwei Yue, Luocong Wang, Haohao Wang, Jirui Du, **Ming Lei***, Min Pu* (2022) “First Principles Study

on the Electrocatalytic Oxygen Evolution Reaction on the (110) Surfaces of Layered Double Hydroxides." J. Phys. Chem. C, 126(43): 18351-18365

150. Xuehui Liu, Haohao Wang, Weidan Li, Jiawen Chen, Jiaqi Fang, Xiaoying Yan, Shuo Mi, Song Hong, **Ming Lei**, Xiong Yin*, Lu Bai, Yanjun Guo*, Rui Xu, Zhihai Cheng*, Leyu Wang* (2022) "Molybdenum-Single Atom Catalyst for High-Efficiency Cobalt(III)/(II)-Mediated Hybrid Photovoltaics." ACS Appl. Energy Mater., 5(10): 12991-12998
149. Peihuan Zhang, Zhewei Li, Yangqiu Liu, Fuxing Shi, Luocong Wang, Min Pu*, **Ming Lei*** (2022) " Hydride Relay Exchange Mechanism for the Heterocyclic C–H Arylation of Benzofuran and Benzothiophene Catalyzed by Pd Complexes." J. Org. Chem., 87(19): 12997-13010
148. Haohao Wang, Fuxing Shi, Min Pu, **Ming Lei*** (2022) " Theoretical Study on Nitrobenzene Hydrogenation by N-Doped Carbon-Supported Late Transition Metal Single-Atom Catalysts." ACS Catal., 12(18): 11518-11529
147. Xinyuan Liu‡, Fuxing Shi‡, Chaochao Jin, Binbin Liu, **Ming Lei***, Jiajing Tan* (2022) "Stereospecific Synthesis of Monofluoroalkenes and Their Deuterated Analogues via Ag-Catalyzed Decarboxylation." J. Catal., 413(2022): 1089-1097 (‡ equal contribution)
146. Zhewei Li, Huili Zhang*, Tianwei Tan*, **Ming Lei*** (2022) " The Mechanism of Direct Reductive Amination of Aldehyde and Amine with Formic Acid Catalyzed by Boron Trifluoride Complexes: Insights from a DFT Study." Catal. Sci. Tech., 12(18): 5679-5686
145. Fuxing Shi, Xiaochuan Ren, Haohao Wang, Min Pu, Li Liu*, **Ming Lei*** (2022) " Neutral Phosphine-Sulfonate Pd Complex-Catalyzed Copolymerization of 2-Methoxystyrene and Ethylene Polar Monomers: A DFT Mechanistic Study." ACS Appl. Polym. Mater., 4(8): 5901-5908
144. Meng Li‡, Ruixue Zhang‡, Qiushan Gao, Huanfeng Jiang, **Ming Lei***, Wanqing Wu* (2022) "Divergent Synthesis of Fused Tetracyclic Heterocycles from Diarylalkynes Enabled by the Selective Insertion of Isocyanide." Angew. Chem. Int. Ed., 61(42): e202208203 (‡ equal contribution)
143. Yangming Ding‡, Tenglong Guo‡, Zhewei Li‡, Bo Zhang*, Fritz E. Kühn, Chang Liu, Jian Zhang, Dezhu Xu, **Ming Lei***, Tao Zhang, Changzhi Li* (2022) " Transition-Metal-Free Synthesis of Functionalized Quinolines by Direct Conversion of β-O-4 Linkages." Angew. Chem. Int. Ed., 61(38): e202206284 (‡ equal contribution)
142. Yangqiu Liu, Hexiang Qi, **Ming Lei*** (2022) "Elastic Image Pair Method for Finding Transition States on Potential Energy Surfaces Using Only First Derivatives." J. Chem. Theory Comput., 18(8): 5108-5115
141. Hongyuan Fu, Jia Yao, Ming Zhang, Lingwei Xue, Qiuju Zhou, Shangyu Li, **Ming Lei**, Lei Meng, Zhi-Guo Zhang*, Yongfang Li (2022) "Low-cost Synthesis of Small Molecule Acceptors Makes Polymer Solar Cells Commercially Viable." Nat. Commun., 13: 3687
140. Hexiang Qi, Yangqiu Liu, Min Pu, Zuoying Yang, Yaping Li, **Ming Lei*** (2022) " Construction and Practice of Molecular Point Group Virtual Laboratory."Chin. J. Chem. Edu., 43(12): 104-113 (祁鹤翔，刘阳秋，蒲敏，杨作银，李亚平，雷鸣* (2022) "分子点群虚拟仿真实验的建设与实践" 化学教育 43(12): 104-113)
139. Bo Zhang‡, Tenglong Guo‡, Zhewei Li‡, Fritz E. Kühn, **Ming Lei**, Zongbao K. Zhao, Jianliang Xiao, Jian Zhang, Dezhu Xu, Tao Zhang, Changzhi Li* (2022) "Transition-metal-free Synthesis of Pyrimidines from Lignin β-O-4 Segments via a One-pot Multi-component Reaction." Nat. Commun., 13: 3365 (‡ equal contribution)
138. Ying Zhou, Yaqi Zhao, Xiaofan Shi, Yanhui Tang, Zuoyin Yang*, Min Pu, **Ming Lei*** (2022) "Theoretical Study on the Hydrogenation of CO2 to Methanol Catalyzed by Ruthenium Pincer Complexes." Dalton Trans., 51(26): 10020-10028
137. Chenxi Sheng, Zhewei Li, Min Pu*, **Ming Lei*** (2022) " Theoretical Study on the Mechanism of the Benzaldehydes Deoxyfluorination by Sulfuryl Fluoride and Tetramethylammonium Fluoride." J. Phys.

Org. Chem., 35(8): e4389

136. Yaqi Zhao, Lin Zhang, Yanhui Tang, Min Pu*, **Ming Lei*** (2022) “Theoretical Study on Asymmetric Ketone Hydrogenation Catalyzed by Mn Complexes: From the Catalytic Mechanism to the Catalyst Design.” Phys. Chem. Chem. Phys., 24(21): 13365-13375
135. **Ming Lei** ‡, Xingyu Chen ‡, Yingjie Wang ‡, Liran Zhang, Hong Zhu*, Zhiqian Wang* (2022) “Homogeneous and Heterogeneous Pd-Catalyzed Selective C–P Activation and Transfer Hydrogenation for “Group-Substitution” Synthesis of Trivalent Phosphines.” Org. Lett., 24(15): 2868-2872 (‡ equal contribution)
134. Luocong Wang, Zhewei Li, Caiwei Yue, Peihuan Zhang, **Ming Lei***, Min Pu* (2022) “Theoretical Study on the Isomerization Mechanism of Azobenzene Derivatives under Electric Field.” Acta Chim. Sinica, 80(6): 781-787 (王珞聪, 李哲伟, 岳彩巍, 张培焕, 雷鸣*, 蒲敏* (2022) “电场下偶氮苯衍生物分子顺反异构化反应机理的理论研究” 化学学报 80(6): 781-787)
133. Lin Zhang, Yaqi Zhao, Chong Liu, Min Pu, **Ming Lei***, Zexing Cao* (2022) “Hydroboration of CO2 to Methyl Boronate Catalyzed by a Manganese Pincer Complex: Insights into the Reaction Mechanism and Ligand Effect.” Inorg. Chem., 61(14): 5616–5625
132. Zhuo Quan, Li Mao, Yi-Qi Tang, **Ming Lei**, Ben-Zhan Zhu*, Ya-Jun Liu* (2022) “Mechanistic Investigation of H2O2-dependent Chemiluminescence from Tetrabromo-1,4-Benzoquinone.” ChemPhysChem, 23(5): e202100885
131. Rui Wang, Yangqiu Liu, Qianyue Wang, Lin Zhang, Zhewei Li, Min Pu*, **Ming Lei*** (2021) “The Role of AQ in the Regioselectivity of Strong Alkyl C–O Bond Activation Catalyzed by Pd(OAc)2: A Density Functional Theory Mechanistic Study.” Inorg. Chem., 60(23): 17555–17564
130. Chong Liu, Lin Zhang, Longfei Li*, **Ming Lei*** (2021) “Theoretical Design of a Catalyst with Both High Activity and Selectivity in C–H Borylation.” J. Org. Chem., 86(23): 16858–16866
129. Hong Yan*, Yi Yang, Tao Wang, Jun Lu, Jing He, Yongmei Chen, Jiaxi Xu, Shouli Bai, Zhihua Wang, **Ming Lei** (2021) “Promoting the Construction of First-Class Applied Chemistry Major by Optimizing the Elements of Students’ Cultivation.” Univ. Chem., 36(11): 2107085 (鄢红*, 杨屹, 王涛, 陆军, 何静, 陈咏梅, 许家喜, 白守礼, 王志华, 雷鸣 (2021) “着力优化育人要素，全面促进应用化学一流本科专业建设” 大学化学 36(11): 2107085)
128. Yaqi Zhao, Lin Zhang, Zhewei Li, Min Pu*, **Ming Lei*** (2021) “Theoretical Study on the Mechanism of C-N and C-C Coupling to Form Indole Catalyzed by Pd(OAc)2.” Mol. Catal., 515: 111895
127. Yaqi Zhao, Lin Zhang, Min Pu*, **Ming Lei*** (2021) “A Phosphine-Free Mn(I)-NNS Catalyst For Asymmetric Transfer Hydrogenation of Acetophenone: A Theoretical Prediction.” Dalton Trans., 50(41): 14738-14744
126. Fuxing Shi, Xiaolin Li, Yinna Bai, Longfei Li, Min Pu, Li Liu*, **Ming Lei*** (2021) “Mechanism of the Zinc Dithiocarbamate-Activated Rubber Vulcanization Process: A Density Functional Theory Study.” ACS Appl. Polym. Mater., 3(10): 5188–5196
125. Haohao Wang, Wei Zhang, Yangqiu Liu, Min Pu*, **Ming Lei*** (2021) “First-Principles Study on the Mechanism of Nitrobenzene Reduction to Aniline Catalyzed by a N-Doped Carbon-Supported Cobalt Single-Atom Catalyst.” J. Phys. Chem. C, 125(35): 19171-19182
124. Ling Zhu ‡, Lin Zhang ‡, Zuoyin Yang, Min Pu*, **Ming Lei*** (2021) “Theoretical Study on the Hydroboration of α, β-Unsaturated Carbonyl Compounds Catalyzed by Metal-Free Complex and Subsequent C−C Coupling with Acetonitrile.” New J. Chem., 45(31): 14134-14140 (‡ co-first author)
123. Yifan Ping, Rui Wang‡, Qianyue Wang‡, Taiwei Chang, Jingfeng Huo, **Ming Lei***, Jianbo Wang* (2021) “Synthesis of Alkenylboronates from N-Tosylhydrazones through Palladium-Catalyzed Carbene Migratory Insertion.” J. Am. Chem. Soc., 143(26): 9769–9780 (‡ equal contribution)
122. Yuting Tao, Jinjiang Xu, Haobin Zhang, Zuoyin Yang, **Ming Lei***, Jie Sun*(2021) “Thermal Expansion

Characteristic of a New Type High Energy Explosive ICM-101." Chinese J. Energetic Materials, 29(7): 641-649 (陶玉婷, 徐金江, 张浩斌, 杨作银, 雷鸣*, 孙杰* (2021)"新型高能量密度炸药ICM-101的热膨胀特性" 含能材料 29(7): 641-649)

121. Xin Xu‡, Lin Zhang‡, Haoqiang Zhao‡, Yixiao Pan, Jiajie Li, Zhenli Luo, Jiahong Han, Lijin Xu*, **Ming Lei*** (2021) "Cobalt(III)-Catalyzed Regioselective C6 Olefination of 2-Pyridones Using Alkynes: Olefination/Directing Group Migration and Olefination." Org. Lett., 23(12): 4624–4629 (‡ Co-first author)
120. Yuting Tao‡, Jinjiang Xu‡, Haobin Zhang, Shiliang Huang, Zuoyin Yang*, Jie Sun*, **Ming Lei*** (2021) "Experimental and Theoretical Study on the Growth of Plate-like β-HMX Crystals in the Hydroxylated Interlayer Space." Phys. Chem. Chem. Phys., 23(21): 12340-12349 (‡ Co-first author)
119. Xin Xu‡, Chenguang Luo‡, Haoqiang Zhao‡, Yixiao Pan, Xin Zhang, Jiajie Li, Lijin Xu*, **Ming Lei***, Patrick Joseph Walsh* (2021) "Rhodium(III)-Catalyzed C–H bond Functionalization of 2-Pyridones with Alkynes: Switchable Alkenylation, Alkenylation/Directing Group Migration and Rollover Annulation." Chem. Eur. J., 27(34): 8811-8821(‡ Co-first author)
118. Lin Zhang, Min Pu, **Ming Lei*** (2021) "Hydrogenation of CO2 to Methanol Catalyzed by Manganese Pincer Complex: Insights on Mechanism and Solvent Effect." Dalton Trans., 50(21): 7348-7355
117. Lin Zhang, Bin Wang, Yaqi Zhao, Min Pu, Shubin Liu*, **Ming Lei*** (2021) "Using Bases as Initiators to Isomerize Allylic Alcohols: Insights from Density Functional Theory Studies." J. Phys. Chem. A, 125(11): 2316–2323
116. Peihuan Zhang, Yufeng Zhang, Zhewei Li, Yang Gao, **Ming Lei**, Zuoyin Yang, Min Pu* (2021) "Theoretical Investigation of Prolyl–Histidine–catalyzed Intermolecular Aldol Reaction." J. Phys. Org. Chem., 34(8): e4203
115. Zhewei Li, Lin Zhang, Min Pu, **Ming Lei*** (2021) "Mechanistic Understanding on Base–catalyzed Aldimine/Ketamine Condensations: An Old Story and A New Model." Asian J. Org. Chem., 10(3): 634-641
114. Ju Wang*, **Ming Lei***, Zhaoxu Wang, Yusheng Liu, Wenchang Zhuang, Wenyou Zhu (2021) "Methanol Oxidation over Rutile Au1@TiO2 Catalyst: Importance of Facets and Oxygen Vacancy." Appl. Surf. Sci., 542 (2021): 148541
113. Lintao Bai, Mingkun Wang, Lin Zhang, Meijun Zhao, Mei Ren, Lirong Zheng, **Ming Lei**, and Heyun Shen* (2021) "Poly(Amino Acid) Coordination Nanoparticle as a Potent Sonosensitizer for Cancer Therapy." ACS Appl. Bio Mater., 4(1): 881-889
112. Yinxing Zou‡, Zhewei Li‡, Yangqiu Liu, **Ming Lei*** (2021) "Is the Eclipsed Conformation of Ethane a Transition State?" Chin. J. Chem. Edu., 42(2): 80-83 (邹寅星‡, 李哲伟‡, 刘阳秋, 雷鸣* (2021) "重叠式乙烷构象是过渡态吗？" 化学教育 42(2): 80-83 (‡ Co-first author))
111. Xiaoliang Liu, Yangqiu Liu, and **Ming Lei***(2021)"A Web-Based Point Group Teaching Platform (PGLite) in Structural Chemistry Course." Univ. Chem., 36(2): 1912065 (刘晓亮, 刘阳秋, 雷鸣* (2021) "结构化学课程中基于网络的点群演示教学平台PGLite的开发与实践" 大学化学 36(2): 1912065)
110. Xiaomin Hu, Yutian Yu, Siyu Chen, **Ming Lei**, Min Pu, Zuoyin Yang* (2020) "Hydrogen Bond Cooperative Effect in Single Cage Water Clusters." Chin. J. Struct. Chem., 39(7): 1213-1225
109. Ruiqin Ding‡, Jinjiang Xu‡, Yuting Tao, Jie Sun*, **Ming Lei*** (2020)"Experimental and Theoretical Study on the Stability of CL-20 Based Host-Guest Energetic Materials." J. Phys. Chem. A, 124(31): 6389–6398 (‡ Co-first author)
108. Wenfang Xiong‡, Fuxing Shi‡, Ruixiang Cheng, Baiyao Zhu, Lu Wang, Pengquan Chen, Hongming Lou, Wanqing Wu, Chaorong Qi*, **Ming Lei***, Huanfeng Jiang* (2020) "Palladium-Catalyzed Highly Regioselective Hydrocarboxylation of Alkynes with Carbon Dioxide."ACS Catal., 10(14): 7968–7978 (‡ Co-first author)

107. Yangqiu Liu, Xin Yue, Longfei Li, Zhewei Li, Lin Zhang, Min Pu, Zuoyin Yang, Chao Wang, Jianliang Xiao*, **Ming Lei*** (2020) “Asymmetric Induction with a Chiral Amine Catalyzed by a Ru-PNP Pincer Complex: Insight from Theoretical Investigation.” Inorg. Chem., 59(12): 8404-8411
106. Wei Zhang, Min Pu, **Ming Lei*** (2020) “Theoretical Studies on Stability and Reactivity of Metals Doped CeO2(100) surface: Towards H2 Dissociation and Oxygen Vacancy Formation.” Langmuir, 36(21): 5891–5901
105. Kun Wang, Lin Zhang, Weijun Tang, Huaming Sun, Dong Xue, **Ming Lei**, Jianliang Xiao, Chao Wang* (2020) “Asymmetric Guerbet Reaction to Access Chiral Alcohols.” Angew. Chem. Int. Ed., 59(28): 11408-11415
104. Zhewei Li, Qianyue Wang, Min Pu*, Zuoyin Yang, **Ming Lei*** (2020) “Theoretical Study on Nitrogenous Heterocyclic Assisted Aldimine Condensation.” Acta Chim. Sinica, 78(5):437-443 (李哲伟, 王骞阅, 蒲敏*, 杨作银, 雷鸣* (2020) “含氮杂环协助的醛胺缩合反应机理的研究” 化学学报 78(5):437-443)
103. **Ming Lei***, Zuoyin Yang, Yaping Li, Min Pu (2020) “Online Teaching of Structural Chemistry Course Based on “1 + 2” Platform.” Univ. Chem., 35(5):98-103 (雷鸣*, 杨作银, 李亚平, 蒲敏 (2020) “基于“1 + 2”模式的结构化学课程在线教学实践” 大学化学 35(5):98-103)
102. Xiaomin Hu, Yutian Yu, Siyu Chen, **Ming Lei**, Min Pu, Zuoyin Yang* (2020) “Relationship between types of central water molecule pairs in single cage water cluster.” J. Mol. Sci., 36(171):30-34 (胡晓敏, 余雨田, 陈思宇, 雷鸣, 蒲敏, 杨作银* (2020) “单笼形水分子簇中心水分子对类型关系” 分子科学学报 36(171):30-34)
101. Chenguang Luo, Longfei Li, Xin Yue, Pengjie Li, Lin Zhang, Zuoyin Yang, Min Pu, Zexing Cao*, **Ming Lei*** (2020) “ pH-Dependent transfer hydrogenation or dihydrogen release catalyzed by a [(h6-arene)RuCl(k2-N,N-dmobpy)]+ complex: a DFT mechanistic understanding.” RSC Adv., 10:10411–10419
100. Chenguang Luo, Lin Lu, Lin Zhang, Zuoyin Yang, Min Pu, Biaolin Yin,* **Ming Lei***(2020) “Transition-Metal-Free Polycyclic Indoles Formation via A Free Radical Pathway: A Computational Mechanistic Study.” Thero. Chem. Acc., 43
99. Ju Wang,* Wei Zhang, Wenyou Zhu, Wenchang Zhuang, **Ming Lei** (2020) “Rutile TiO2 supported single atom Au catalyst: A facile approach to enhance methanol dehydrogenation.” Mol. Catal., 482:110670
98. Ruiqin Ding, Yuting Tao, Jinjiang Xu, Jie Sun,* **Ming Lei*** (2020) “Review on Crystal Structure and Properties of Energetic Compound CL-20 and Its Cocrystals .” J. WuHan Univ. (Natural Sci. Ed.), 1:23-31 (丁瑞琴, 陶玉婷, 徐金江, 孙杰,* 雷鸣* (2020)“含能化合物C L-20及其共晶的结构及性能研究进展” 武汉大学学报(理学版) 1:23-31)
97. Zheliang Cao, Wei Zhang, Ruiqin Ding, Ju Wang, Min Pu, Zuoyin Yang, **Ming Lei*** (2020) “The reaction paths of CH2O decomposition on CuO(111) surface: A DFT study.” J. Phys. Org. Chem., 33(1):e4017
96. Yangqiu Liu, Xin Yue, Chenguang Luo, Lin Zhang, **Ming Lei*** (2019) “Mechanisms of Ketone/Imine Hydrogenation Catalyzed by Transition-Metal Complexes.” Energy Environ. Mater., 2(4):292-312
95. Lin Zhang, Wei Zhang, Xin Yue, Pengjie Li, Zuoyin Yang, Min Pu, **Ming Lei*** (2019) “Theoretical Study on Mechanism of CO2 Hydrogenation to Formic Acid Catalyzed by Manganese Complex.” Chem. J. Chinese Univ., 40(9):1911-1917.
94. Qianyue Wang, Longfei Li, Pengjie Li, Xin Yue, Zuoyin Yang, Min Pu, **Ming Lei*** (2019) “Ruthenium-catalyzed deoxygenative hydroboration of carboxylic acids: a DFT mechanistic study.” New J. Chem., 43:11493-11496
93. Xin Yue, Longfei Li, Pengjie Li, Chenguang Luo, Min Pu, Zuoyin Yang, **Ming Lei*** (2019) “ A Computational Study on Iridium‐Catalyzed Production of Acetic Acid from Ethanol and Water Solution.” Chinese J. Chem., 37 (9):883-886
92. Miao Xiao,# Xin Yue,# Ruirui Xu, Weijun Tang, Dong Xue, Chaoqun Li, **Ming Lei**,* Jianliang Xiao,* Chao

Wang* (2019) “Transition‐Metal‐Free Hydrogen Autotransfer: Diastereoselective N‐Alkylation of Amines with Racemic Alcohols.” Angew. Chem. Int. Ed., 58 (31):10528-10536 (# Co-first author)

91. Wei Zhang, Xuelu Ma, Hai Xiao, **Ming Lei**,* Jun Li* (2019) “Mechanistic Investigations on Thermal Hydrogenation of CO2 to Methanol by Nanostructured CeO2(100): The Crystal-Plane Effect on Catalytic Reactivity.” J. Phys. Chem. C, 123 (18):11763-11771
90. Qinghong Xu, Jiali Liang, Xu Teng, Xin Yue, **Ming Lei**, Caifeng Ding, Chao Lu* (2019) ”Rapid screening of the hydrogen bonding strength of radicals by electrochemiluminescent probes.” Chem. Commun., 55:5563-5566
89. Lin Lu, Chenguang Luo, Hui Peng, Huanfeng Jiang, **Ming Lei**, Biaolin Yin* (2019) ”Access to Polycyclic Sulfonyl Indolines via Fe(II)-Catalyzed or UV-Driven Formal [2+2+1] Cyclization Reactions of N-((1H-indol-3-yl)methyl)propiolamides with NaHSO3.” Org. Lett., 21 (8):2602-2605
88. Jialuo She, Xiangfeng Lin, Zaihui Fu,* Jianwei Li,* Senpei Tang, **Ming Lei**, Xin Zhang, Chao Zhang, Dulin Yin (2019) “HCl and O2 co-activated bis(8-quinolinolato) oxovanadium(IV) complexes as efficient photoactive species for visible light-driven oxidation of cyclohexane to KA oil.” Catal. Sci. Tech., 9: 275-285
87. Jialing Ma, Hui Zhang, Xin Zhang,* **Ming Lei*** (2019) “3D-QSAR studies of D3R antagonists and 5-HT1AR agonists.” J. Mol. Graph. Model., 86:132-141
86. Pei-Huan Zhang, Min Pu,* Yang Gao, Yu-Feng Zhang, **Ming Lei**, Zuo-Yin Yang (2018) “Theoretical Study of the Histidine-catalyzed Asymmetric Aldol Reaction of Acetone and Benzaldehyde.” J. Phys. Chem. A, 122(39): 7842-7851
85. Yutian Yu, Xiaomin Hu, **Ming Lei**, Zuoying Yang* (2018). “The relationship between water molecule pairs and hydrogen bond energy in cage hydration clusters.” Journal of Beijing Univ. of Chem. Tech., 45(6): 6-12
84. Pengjie Li, Longfei Li, Xin Yue, Qianyue Wang, Min Pu, Zuoyin Yang, **Ming Lei*** (2018) “1,2 addition or cycloaddition of allenes by a dihafnium μ−Nitrido complex? A DFT study.” J. Organomet. Chem., 874: 101-105
83. Longfei Li, **Ming Lei**,* Li Liu,* Yaoming Xie, Henry F. Schaefer III* (2018) “Metal‐Substrate Cooperation Mechanism for Dehydrogenative Amidation Catalyzed by a PNN-Ru Catalyst.” Inorg. Chem., 57 (15): 8778-8787
82. Longfei Li, **Ming Lei**,* Yaoming Xie, Frank Weinhold, Henry F. Schaefer III* (2018) “Quantitative Theoretical Predictions and Qualitative Bonding Analysis of the Divinylborinium System and Its Al, Ga, In, and Tl Congeners.” Inorg. Chem., 57(13): 7851-7859
81. Chen-Xi Wang, Min Pu,* Pei-Huan Zhang, Yang Gao, Zuo-Yin Yang, **Ming Lei** (2018) “Structure Simulation and Host‐Guest Interaction of Histidine-Intercalated Hydrotalcite‐Montmorillonite Complex.” Minerals, 8, 198 DOI:10.3390/min8050198
80. Wei Zhang, Yiwei Zhang, Hui Li, **Ming Lei*** (2018) ” Theoretical Study on the Formation Mechanism of Catalytic Active Components in Suzuki-Miyaura Cross-Coupling Reaction Catalyzed by Transition Metal Cobalt Complexes.” Chem. J. Chinese Univ., 39(4): 721-728
79. Longfei Li, Huajie Zhu, Li Liu, Datong Song,* **Ming Lei*** (2018) “A Hydride-Shuttle Mechanism for the Catalytic Hydroboration of CO2.” Inorg. Chem., 57: 3054−3060
78. Pengjie Li, Yanxia Xi, Longfei Li, Hui Li, Wen-Hua Sun,* **Ming Lei*** (2018) “A DFT study on ring-opening polymerization of e-caprolactone initiated by Mg and Al complexes.” Inorg. Chim. Acta, 477(2018): 34-39
77. Hai-Xia Wang*,Wan-Qin Wang, Min Pu, **Ming Lei**, Xiang-Dong Wang (2017) “The Application of Flipped Classroom Mode in the Experimental Teaching of Photometric Determination of Iron.” Univ. Chem., 32(6): 13-17 (王海霞*, 王婉秦, 蒲敏, 雷鸣, 王向东 (2017) “翻转课堂模式在光度法测铁实验教学中的应

用” 大学化学 32(6): 13-17

76. Longfei Li, **Ming Lei**,* Shigeyoshi Sakaki* (2017) “DFT Mechanistic Study on Alkene Hydrogenation Catalysis of Iron Metallaboratorene: Characteristic Features of Iron Species.” Organometallics, 36(18): 3530–3538
75. Longfei Li, **Ming Lei**,* Yaoming Xie, Henry F. Schaefer III,* Bo Chen, Roald Hoffmann* (2017) “Stabilizing a different cyclooctatetraene stereoisomer.” Proc. Natl. Acad. Sci. USA, 114(37): 9803-9808
74. Xuelu Ma, **Ming Lei*** (2017) ”Mechanistic Insights into the Directed Hydrogenation of Hydroxylated Alkene Catalyzed by Bis(phosphine)cobalt Dialkyl Complexes.” J. Org. Chem., 82(5): 2703-2712
73. Jing Wang, Lei He, Feng Nan, Fan Wang, Hongming Li, Jingjiang Wang, Dong Liu, **Ming Lei**, Longfei Li, Qigu Huang,* Wantai Yang (2017) ”Investigation on terpolymer of ethylene/propylene/ ω -bromo- α -olefins catalyzed by titanium complexes.” J. Mater. Sci., 52(10):5981-5991
72. Hao Cao, Yang Jiang, Haiyang Zhang, Kaili Nie, **Ming Lei**, Li Deng,* Fang Wang, Tianwei Tan* (2017) ”Enhancement of methanol resistance of Yarrowia lipolytica lipase 2 using β -cyclodextrin as an additive: Insights from experiments and molecular dynamics simulation.” Enzyme Microb. Tech., 96:157-162
71. Hao Cao, Meng Wang, Kaili Nie, Xin Zhang, **Ming Lei**, Li Deng,* Fang Wang, Tianwei Tan (2017) ”β -cyclodextrin as an additive to improve the thermostability of Yarrowia lipolytica Lipase 2: Experimental and simulation insights.” J. Taiwan Inst. Chem. E, 70:49-55
70. Yanxia Xi, Natesan Mannangatti Rajendran, Wenjuan Zhang, Yang Sun, **Ming Lei**, Wen-Hua Sun* (2016) ”Quinolyl-amidinates Chelating Bimetallic Magnesium and Mononuclear Aluminum Complexes for ε -Caprolactone Polymerization.” ChemistrySelect 1: 5660-5665
69. Hui Li, Xuelu Ma, Baohua Zhang, **Ming Lei*** (2016) ”DFT Study on the Mechanism of Tandem Oxidative Acetoxylation/Ortho C–H Activation/Carbocyclization Catalyzed by Pd(OAc)2.” Organometallics 35(19): 3301-3310
68. Hui Li, Xuelu Ma, **Ming Lei*** (2016) ”Substituent Effects and Chemoselectivity in the Intramolecular Buchner Reaction of Diazoacetamide Derivatives Catalyzed by Di-Rh(II)-Complex .” Dalton Trans., 45: 8506-8612
67. Yiwei Zhang, Xuelu Ma, Xin Zhang,* **Ming Lei*** (2016) ”Theoretical Study on N-N Activation by Thiolate-bridged Dinuclear Dinitrogen Transition-metal Complexes.” Acta Chim. Sinica, 74(4): 340-350
66. Xinli Duan, Xin Zhang,* Binglin Xu, Fang Wang, **Ming Lei*** (2016) ”Theoretical Study and Modified Design of Selective Dopamine D3 Receptor Agonists.” Chem. Biol. Drug Des., 88: 142-154
65. Longfei Li, Yuhui Pan, **Ming Lei*** (2016) ”The Enantioselectivity in Asymmetric Hydrogenation of Ketone Catalyzed by Ru-Binap Complex: Insights From a 3D-QSSR to DFT Study.” Catal. Sci. Technol., 6: 4450-4457
64. Xinli Duan, Xin Zhang,* **Ming Lei*** (2015) ”Mechanisms for the Hydrolytic Deamination of Nicotinamidase: a QM/MM MD Understanding.” Chem J Chinese U 36(12):2491-2496
63. Longfei Li, Yinna Bai, **Ming Lei**,* Li Liu* (2015) ”Progress in Rubber Vulcanization Accelerator.” Prog Chem 10:1500-1508 (Review in Chinese)
62. Xuelu Ma, **Ming Lei**,* Shubin Liu* (2015) ”Homolytic or Heterolytic Dihydrogen Splitting with Bimetallic Dinitrogen Complexes? A Computational Study.” Organometallics 34(7): 1255-1263
61. Xinli Duan, Min Zhang, Xin Zhang, Fang Wang,* **Ming Lei*** (2015) “Molecular Modeling and Docking Study on Dopamine D2-likeand Serotonin 5HT2A Receptors.” J Mol Graph Model 57:143-155
60. **Ming Lei**,* Yuhui Pan, Xuelu Ma (2015) ”The nature of hydrogen production from aqueous-phase methanol dehydrogenation with ruthenium pincer complexes under mild conditions.” Eur J Inorg Chem 5: 794-803
59. Hao Cao, Li Deng,* **Ming Lei**,* Fang Wang, Tianwei Tan (2014) “The Role of Temperature and Solvent

on the Activity of Yarrowia Lipase 2: Insights From Molecular Dynamic Simulation." J Mol Catal B 109:101-108

58. Xuelu Ma, Yanhui Tang, **Ming Lei*** (2014) " Bent and Planar Structures of μ-η2, η2-N2 Dinuclear Early Transition Metal Complexes." Dalton Trans 43 (30):11658-11666
57. **Ming Lei***, Zhidong Wang, Xiaojie Du, Xin Zhang, Yanhui Tang (2014) " Asymmetric Hydroformylation Catalyzed by Rh(YANPHOS)H(CO)2: Mechanism and Origin of Enantioselectivity." J Phys Chem A 118(39): 8960-8970
56. Min Wang, Xin Zhang,* Zhuo Chen, Yanhui Tang, **Ming Lei*** (2014) " A DFT Study of Mechanism of Intermolecular Hydroacylation of Aldehyde and Ketone." Sci China Chem 57(9):1264-1275
55. Qintian Ma, Qingyuan Yang,* Aziz Ghoufi, Ke Yang, **Ming Lei**, Gerard Ferey, Chongli Zhong, Guillaume Maurin* (2014) " Guest-modulation of the mechanical properties of flexible porous metal–organic frameworks." J Mater A 2: 9691-9698
54. Lijun Zhao, **Ming Lei*** (2014) "Progress in computational chemical studies on transthyretin." Prog Chem 26(1):193-202 (Review, in Chinese)
53. Xin Zhang, **Ming Lei*** (2013) " Which is the Proton-shuttle in Isoxanthopterin Deaminase? QM/MM MD Understanding." J Theor Comput Chem 12(8):1341002 DOI: 10.1142/S0219633613410022
52. Xiaojie Du, Yanhui Tang, Xin Zhang, **Ming Lei*** (2013) " A Theoretical Study on the Alkene Insertion Step in Rh-Yanphos Catalyzed Hydroformylation." Chinese Chem Lett 24(12):1083-1086link
51. Lijun Zhao, Liangren Zhang, **Ming Lei*** (2013). " A 3D-QSAR and Docking Study on Transthyretin Amyloidgenesis Inhibitors." Sci China Chem 56(11):1550-1563
50. Xuelu Ma, Yanhui Tang, **Ming Lei*** (2013) "Mechanistic Studies on the Carboxylation of Hafnocene and Aansa-zirconocene Dinitrogen Complexes with CO2." Organometallics 32(23):7077-7082
49. Xuelu Ma, **Ming Lei*** (2013) " Progress in Dinitrogen Fixation Activated by Binuclear Transition-Metal Complexes." Prog Chem 25(8):1325-1333 (Review, in Chinese)
48. Xuelu Ma, Xin Zhang, Wenchao Zhang, **Ming Lei*** (2013) " CO Assisted N2 Functionalization Activated by Dinuclear Hafnium Complex: A DFT Mechanistic Exploration." Phys Chem Chem Phys 15(3): 901-910
47. Ran Feng,¶ Ang Xiao,¶ Xin Zhang,* Yanhui Tang, **Ming Lei*** (2013) " Origins of Stereoselectivity in the Hydrogenation of Ketones Catalyzed by Ru Catalyst: Insights from a Computational Study." Dalton Trans 42(6):2130-2145 (¶ Co-first author)
46. Mawia Hessan, Xin Zhang,* Wenchao Zhang, Biaohua Chen, **Ming Lei*** (2012) "How the Methanol Assists the Hydrogen Transfer in Pd-catalyzed Cyclocarbonylation of Allylic Alcohols? Insights from a DFT Study." Chem Lett 41 (7): 693-695
45. Tianhu Yuan, Xin Zhang, Zehan Hu, Fang Wang*, **Ming Lei*** (2012). "Molecular Dynamics Studies of the Antimicrobial Peptides Piscidin 1 and Its Mutants with a DOPC Lipid Bilayer." Biopolymers 97 (12): 998-1009
44. Xin Zhang, Xiaojia Guo, Yue Chen, **Ming Lei**,* Weihai Fang* (2012). "Mechanism investigation of ketone hydrogenation catalyzed by ruthenium bifunctional catalysts: insights from a DFT Study." Phys. Chem. Chem. Phys. 2012, 14 (17): 6003-6012
43. Wenchao Zhang, Yanhui Tang, **Ming Lei**,* Keiji Morokuma, Djamaladdin G. Musaev* (2011) "Ditantalum Dinitrogen complex: On reaction of H2molecule with an "End-on-bridged" [TaIV]2(μ-η1: η1-N2) and Bis(μ-nitrido) [TaIV]2(μ-N)2 complexes." Inorg Chem 50(19): 9481–9490
42. Xiaojia Guo, Yanhui Tang, Xin Zhang, **Ming Lei*** (2011) " Concerted or Stepwise Hydrogen Transfer in the Transfer Hydrogenation of Acetophenone Catalyzed by Ruthenium-Acetamido Complex? A Theoretical Mechanistic Investigation" J Phys Chem A 115(44): 12321-12330
41. Xin-Tian Feng, Jian-Guo Yu, Ruo-Zhuang Liu, **Ming Lei**, Wei-Hai Fang, Frank De Proft, Shubin Liu

(2010) ” Why Iron? A Spin-Polarized Conceptual Density Functional Theory Study on Metal-Binding Specificity of Porphyrin.” J Phys Chem A 114(21):6342-6349

40. Zhuo Chen, Yue Chen, Yanhui Tang, **Ming Lei*** (2010) “A Theoretical Study of X Ligand Effect on Catalytic Activity of the Complexes RuHX(diamine)(PPh3)2 (X = NCMe, CO, Cl, OMe, OPh, CCMe, H) in H2-hydrogenation of Ketones.” Dalton Trans 39:2036-2043
39. **Ming Lei**,* Wenchao Zhang, Yue Chen, Yanhui Tang (2010) ” Preference of H2 as Hydrogen Source in Hydrogenation of Ketone Catalyzed by Late Transition Metal Complexes.” Organometallics 29(3):543-548
38. Xin-Tian Feng, Jian-Guo Yu, **Ming Lei**, Wei-Hai Fang, Shubin Liu (2009). “Toward Understanding Metal-Binding Specificity of Porphyrin: A Conceptual Density Functional Theory Study.” J Phys Chem B 113(40):13381-13389
37. Baohua Zhang, Tianhu Yuan, Hua Jiang,* **Ming Lei*** (2009). ” Molecular Dynamics Simulations on the Stability and Assembly Mechanisms of Quadruple and Double Helical Aromatic Amide Foldamer.” J Phys Chem B 113(31):10934-10941
36. Yue Chen, Yanhui Tang, Shubin Liu, **Ming Lei***, Weihai Fang* (2009). “Mechanism and Influence of Acid in H2-hydrogenation of ketones catalyzed by η6-Arene/N-Tosylethylenediamine-Ruthenium(II).” Organometallics 28(7):2078–2084
35. Yue Chen, Yanhui Tang, **Ming Lei*** (2009). “A Comparative Study on Hydrogenation of Ketone Catalyzed by Diphosphine-diamine Transition Metal Complexes using DFT Method.” Dalton Trans 13:2359-2364
34. Ying Liu, Fang Wang, Tianwei Tan, **Ming Lei** (2008). “Rational Design and Study on Recognition Property of Paracetamol-Imprinted Polymer.” Appl Biochem Biotech
33. Aiguo Zhong, Dingben Chen, **Ming Lei***, Shubin Liu* (2008). ” Understanding the Role of Water in Promoting E-isomer Production and Photochromism of Solid Schiff Base: A DFT and TD-DFT Study.” J Theor Comp Chem 7(5): 1071-1084
32. Zehan Hu, Yanhui Tang, Houfang Wang, Xu Zhang, **Ming Lei*** (2008). ” Dynamics and cooperativity of Trp-cage folding.” Arch Biochem Biophys 475(2): 140-147
31. Yue Chen, Shubin Liu*, **Ming Lei*** (2008). “Nature of Asynchronous Hydrogen Transfer in Ketone Hydrogenation Catalyzed by Ru Complex.” J Phys Chem C 112(35): 13524-13527
30. Guilei Wang, Yue Chen, Aiguo Zhong, Hongguang Du, **Ming Lei*** (2008). “A DFT Study on Formation of Bisaryloxime Ether from Benzaldehyde and Phenoxyamine.” Chem Lett 37(6): 656-657
29. Houfang Wang, Yanhui Tang*, **Ming Lei*** (2007). “Models for binding cooperativities of inhibitors with transthyretin.” Arch Biochem Biophys 466(1): 85-97
28. Ying Liu, Fang Wang, Tianwei Tan, **Ming Lei** (2007). ” Study of the properties of molecularly imprinted polymers by computational and conformational analysis.” Anal Chim Acta 581: 137-146
27. Mingfeng Yang,¶ **Ming Lei**,¶ Boyan Yordanov, Shuanghong Huo (2006) “Peptide-plane can flip in two opposite directions: implication in amyloid formation of transthyretin.” J Phys Chem B 110: 5829-5833 (¶ Co first author)
26. Mingfeng Yang, **Ming Lei**, Shuanghong Huo (2005) “ Initial conformational changes of humantransthyretin under partially denaturing conditions.” Biophysical Journal 89: 433-443
25. **Ming Lei**, Mingfeng Yang, Shuanghong Huo, (2004) “ Intrinsic versus mutation dependent instability/flexibility: A comparative analysis of the structure and dynamics of wild-type transthyretin and its pathogenic variants.” Journal of Structure Biology 148(2): 153-168
24. Hao Maorong, Feng Wenlin, Ji Yongqiang, **Lei Ming** (2004). “ IRC Analysis on the Reaction Paths for Methanol Carbonylation Catalyzed by Rh Complex.” Science in China (Series B) 47(1): 41-49.
23. Mingfeng Yang, **Ming Lei**, Shuanghong Huo (2003). “Why is Leu55–>Pro55 transthyretin variant the most amyloidogenic: insights from molecular dynamics simulation of transthyretin.” Protein Science(12):

1222-1231.

22. Zhang Xinzhuang, Xu Zhengfeng., Ji Yongqiang, Feng WenLin, **Lei Ming** (2003). “Kinetics and ab initio studies of hydrogen abstraction reaction “HNCO+HCO -> NCO+CH2O”.” Chinese Journal of Chemical Physics 16(2): 94-98.
21. Yan Jianming, Lin Yuan, Wei Xianfu, Wang Yanqiao, Yang Lianming, **Lei Ming** (2002). “Evalution of charge transport for organic photoreceptor.” Information Recording Materials. 3(2):13-15
20. Li Huiyin, Feng Wenlin*, Ji Yongqiang, **Lei Ming** (2002). “The reaction path and variational rate constant of the hydrogen abstraction reaction CH2O+O[3P] -> CHO+OH.” Acta Phys. Chim. Sin., 18(5): 446-450.
19. Ji Yongqiang, Feng Wenlin*, Xu Zhengfeng, **Lei Ming** (2002). “MP2 and QCISD study of hydrogen transfer reaction path of the reaction HNCO with carbon-hydrogen radicals CHx (x=1 ~ 3).” Acta Chim. Sin., 60(7): 1167-1172.
18. Ji Yongqiang, Feng Wenlin*, Xu Zhengfeng, **Lei Ming** (2002). “Ab initio study on the mechanism of reaction HNCO+NH2.” Science in China (Series B) 45(4): 365-372.
17. **Lei Ming***, Feng Wenlin, Xu Zhenfeng, Ji Yongqiang, Hao Maorong (2001). “Ab initio Study on the Mechanism of Rhodium-complex Catalyzed Carbonylation of Methanol to Acetic Acid.” Science in China (Series B) 44(5): 465-472.
16. Ji Yongqiang, Feng Wenlin*, Xu Zhengfeng, **Lei Ming**, Hao Maorong (2001). “CH3NO2+X(X = H, OH, CH3, CH2[3B1],O[3P])-> CH2NO2+XH- Transition states structures and potential barriers DFT study of absorption hydrogen reaction.” Acta Chim. Sin., 59(12): 2099-2104.
15. Ji Yongqiang, Feng Wenlin*, Xu Zhengfeng, **Lei Ming** (2001). “Theoretical study of molecular interaction between [CH3ONO2]H+ and R-OH.” J. Beijing Univ. of Chem. Tech. 28(4): 66-69.
14. **Lei Ming***, Feng Wenlin, Xu Zhenfeng (2001). “Theoretical Study on the Mechanisms of Some Elementary Reactions Catalyzed by Modified Carbonyl Cobalt.” Chem. J. Chinese Univ., 22(3): 455-459.
13. Li Yonghong, Hong Sanguo, Feng Wenlin*, **Lei Ming** (2000). “Mechanism for isomerization of 3-hydroxy-2-pyridine imine.” Acta Phys. Chim. Sin., 16(11): 992-996
12. Hongxin Huang*, Xianbiao Zeng, **Lei Ming** (2000). “Surplus function variational quantum Monte Carlo approach: Excited state processing.” J. Chem. Phys., 112(12): 5257-5262.
11. **Lei Ming***, Feng Wenlin, Xu Zhenfeng (2000). “Ab initio Study on the key reactions of hydroformylation cycle by carbonyl cobalt.” Acta Phys-Chim Sin., 16(6): 522-526.
10. **Lei Ming***, Feng Wenlin, Xu Zhenfeng (2000). “A Theoretical Investigation on Regioselectivity of Aromatic Ketones in the addition with Olefin catalyzed by RuH2(CO)(PH3)3.” Science in China (Series B) 43(4): 412-420.
9. **Lei Ming***, Feng Wenlin, Xu Zhenfeng (2000). “A theoretical study on electronic and steric effects of phosphorus ligands in homogeneous catalysts.” J. Beijing Univ. of Chem. Tech. 27(2): 66-69.
8. **Lei Ming***, Feng Wenlin, Xu Zhenfeng (2000). “Ab initio MO Study on the Reaction Mechanism for Carbonyl Insertion Catalyzed by the Carbonyl Cobalt Complex.” Chem. Res. Chinese Univ., 19(1): 31-35.
7. **Lei Ming***, Feng Wenlin, Xu Zhenfeng (2000). “Ab initio MO study of reaction mechanism for carbonyl migration of Co complex.” Chinese Sci. Bulletin 45(13): 1176-1178.
6. Hongxin Huang*, Qingji Xie, Zexing Cao, Zelin Li, Zen Yue, **Lei Ming** (1999). “A novel quantum Monte Carlo strategy: Surplus function approach.” J. Chem. Phys., 110(8): 3703-3707.
5. Wan Yan, Feng Wenlin*, **Lei Ming** (1998). “A theoretical calculation of the rate constant for the isomerization from 1,2-butadiene to 1,3-butadiene.” Science in China (Series B) 14(1): 60-64.
4. **Lei Ming***, Qian Yin, Wan Yan, Feng Wenlin (1998). “Theoretical Study on the thermal Isomerization from 1,2-Butadiene to 2-Butyne.” Chem. J. Chinese Univ., 19(4): 586-590

3. Qian Ying, Feng Wenlin*, **Lei Ming**, Wan Yan, Liu RuoZhuang (1997). "A mechanism study on D-A reaction between 1,3-cyclohexylene to propylnitrile." Chinese J. Chem. Phys., 10(6): 514-518.
2. Feng Wenlin*, **Lei Ming**, Wanyan, Qianyin (1997). "Theoretical study on the thermal isomerization from 1,2-butadiene to 1,3-butadiene." Chinese Chem. Lett., Letters 8: 71-72.
1. Hongxin Huang*, Zexing Cao, **Ming Lei** (1996). " Self-optimizing diffusion quantum Monte Carlo calculation: the singlet-triplet splitting in CH2." J. Mol. Struct. (Theochem), 370: 55-63.

CONFERENCES:

33. **Ming Lei** (2019). Theoretical Study on the Activation of H_2 and CO_2 by Boron-containing Complexes. **Invited Presentation**, The 4th Symposium of Chinese Computational Catalysis Network (C3N-4), Xian-Hanzhong, Shanxi Province, P. R. China.
32. **Ming Lei** (2018). Theoretical Insights into Transition-metal-catalyzed Hydrogenation and Dehydrogenation. **Invited Presentation**, The International Symposium on Chemical Concepts from Theory and Computation (CCTC2018), Changsha, Hunan Province, P. R. China.
31. **Ming Lei** (2018). Theoretical Insights into Transition-metal-catalyzed Hydrogenation and Dehydrogenation. **Invited Presentation**, The International Symposium of Computational Organometallic Chemistry (ICOC2018), Zhengzhou, Henan Province, P. R. China.
30. **Ming Lei** (2018). Theoretical Study on the Activation of H_2 and CO_2 by Boron-containing Compounds. **Invited Presentation**, 2018 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry (WFTCPC2018), Emeishan City, Sichuan Province, P. R. China.
29. **Ming Lei** (2018). A Theoretical Study on C-H Bond Activation of sp^2 C-H by Organometallic Complexes. **Invited Presentation**, The 31st Annual National Meeting of China Chemical Society (CCS2018), Hangzhou, Zhejiang Province, P. R. China.
28. **Ming Lei** (2017). A Metal-Substrate Cooperation Mechanism for the C-N Coupling Dehydrogenation of 2-aminoethanol to Form Cyclic and Linear Peptides Catalyzed by a PNN-Ru Catalyst. **Invited Presentation**, The 8th Asian Pacific Conference on Theoretical & Computational Chemistry (APCTC8), Mumbai, India.
27. **Ming Lei** (2017). A Metal-Substrate Cooperation Mechanism for the C-N Coupling Dehydrogenation of 2-aminoethanol to Form Cyclic and Linear Peptides Catalyzed by a PNN-Ru Catalyst. **Invited Presentation**, The 22nd International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCPXXII), Changsha, Hunan Prov., P. R. China.
26. **Ming Lei** (2017). Origins of Enantioselectivity in Asymmetric Ketone Hydrogenation Catalyzed by Ruthenium Complexes: Insights from a Computational Study. **Invited Presentation**, The 8th National Conference of Molecular Chirality (NCMC2017), Fuzhou, Fujian Prov., P. R. China.
25. **Ming Lei** (2017). Origins of Enantioselectivity in Asymmetric Ketone Hydrogenation Catalyzed by Ruthenium Complexes: Insights from a Computational Study. **Invited Presentation**, The 8th National Conference of Molecular Chirality (NCMC2017), Fuzhou, Fujian Prov., P. R. China.
24. **Ming Lei** (2017). Metal-Substrate Cooperation Mechanism for Dehydrogenative Amidation Reaction Catalyzed by a PNN-Ru Catalyst. **Invited Presentation**, The 13th National Conference of Quantum Chemistry, Dalian, Liaoning Province, P. R. China.
23. **Ming Lei** (2016). Theoretical Insights into Transition-metal-catalyzed CO_2 Hydrogenation and Methanol/Formic Acid Dehydrogenation. **Invited Presentation**, The 7th Cross-strait Theoretical and Computational Chemistry Conference (CTCC-7), Changsha, Hunan Province, P. R. China.
22. **Ming Lei** (2016). Difference in Catalytic Activity of Boryl-Co and Boryl-Ni complexes in Alkene Hydrogenation: Insights from a DFT Mechanistic Investigation. **Invited Presentation**, The 30th Annual

Meeting of Chemical Society of China, Dalian, Liaoning Province, P. R. China.

21. **Ming Lei** (2016). Theoretical Insights into Transition-metal-catalyzed Ketone Hydrogenation and Alcohol Dehydrogenation. **Oral Presentation**, The 7th Asia-Pacific Conference of Theoretical and Computational Chemistry, Kaohsiung, Taiwan, P. R. China.
20. **Ming Lei** (2015). Theoretical Insights into Transition-metal-catalyzed Ketone Hydrogenation and Alcohol Dehydrogenation. **Invited Presentation**, The 3rd Symposium of the Theoretical Chemistry，Beijing, P. R. China.
19. **Ming Lei** (2014). The Methanol Dehydrogenation Catalyzed by Defined Ruthenium Pincer Complex: Insights From A DFT Study. **Invited Presentation**, The International Workshop on Computational Science and Engineering，Hong Kong, P. R. China.
18. **Ming Lei** (2014). A Fundamental Understanding on Mechanism of Methanol Dehydrogenation Catalyzed by Ruthenium Pincer Complex. **Oral Presentation**, The International Symposium on Frontiers of Theoretical and Computational Chemistry，Shenzhen, Guangdong Prov. P. R. China.
17. **Ming Lei** (2013). Theoretical Studies on N_2 Activation and Functionalization Catalyzed by Binuclear Transition-metal Complexes. **Oral Presentation**, The 12th National Computational Chemistry Conference, Suzhou, Jiangsu Prov. P. R. China.
16. **Ming Lei** (2013). CO/CO_2 Assisted N_2 Activation and Functionalization Triggered by Dinuclear Transition-metal Complexes. **Oral Presentation**, The 10th National Physical Organic Chemistry Conference, Hefei, Anhui Prov. P. R. China.
15. **Ming Lei** (2013). Origins of Enantioselectivity and Activity in Asymmetric Ketone Hydrogenation Catalyzed by Transition-metla Complexes. **Oral Presentation**, The 15th Asian Chemical Congress, Singapore.
14. **Ming Lei** (2012). Molecular Dynamics Studies of the Antimicrobial Peptides Piscidin 1 and Its Mutants with a DOPC Lipid Bilayer. **Oral Presentation**, Worldwide Chinese Computational Biology and Molecular Simulation Conference (WCCBMSC 2012), Dalian, P. R. China.
13. **Ming Lei** (2011). Theoretical Studies on N2 Activation and Functionalization Catalyzed by Di-Transitionmetal Complex. **Oral Presentation**, International Conference on Theoretical and High Performance Computational Chemistry (ICT-HPCC 2011), Xi'an, P. R. China.
12. **Ming Lei** (2010). Probing the Nature of Asymmetric Hydrogenation of Ketones Catalyzed by Bifunctional Transitional Metal Catalysts. **Oral Presentation**, BIT's 1st Annual World Congress of Catalytic Asymmetric Synthesis, Beijing, P. R. China.
11. **Ming Lei** (2009). Probing the Nature of Asymmetric Hydrogenation of Ketones Catalyzed by Bifunctional Transitional Metal Catalysts. **Oral Presentation**, The 11st National Conference of Homogenous Catalysis, Changsha, P. R. China.
10. **Ming Lei** (2007). Dynamics and cooperativity of Trp-cage folding. **Oral Presentation**, The 3rd International Conference on Theoretical Chemistry, Molecular Modeling and Life Sciences (ICTCLS 07), Yantai, P. R. China.
9. **Ming Lei** (2007). Insights on cooperativity of Trp-cage folding using molecular dynamic simulations. **Oral Presentation**, The 3rd Asian Pacific Conference on Theoretical & Computational Chemistry (APCTC III), Beijing, P. R. China.
8. **Ming Lei** (2007). Models for binding cooperativities of inhibitors with transthyretin. **Oral Presentation**, The 9th National Computational Chemistry Conference, Chengdu, P. R. China, Chinese Chemical Society.
7. Houfang Wang, Yanhui Tang, **Ming Lei** (2007). Channel conformation changes induced by inhibitors' binding: Molecular dynamics insights from the holo- and apo- forms of transthyretinex **Oral Presentation**, The 3rd International Conference of Molecular Simulations and Applied Informatics

Technologies, Hanzhou, P. R. China.

6. Yanhui Tang, **Ming Lei**, Wenlin Feng (2005). A DFT study on chiral hydrogenation of ketone catalyzed by Ru complex. **Oral Presentation**, The 9th National Quantum Chemistry Conference, Guilin, P. R. China, Chinese Chemical Society.
5. **Ming Lei**, Yanhui Tang, Mingfeng Yang, Shuanghong Huo (2005). Role of conformational change investigated by multiple molecular dynamics simulation of V14N/V16E mutant of transthyretin. **Oral Presentation**, International Symposium on Protein Folding, Function and Dynamics, Beijing, P. R. China
4. **Ming Lei**, Mingfeng Yang, Shuanghong Huo (2004). A comparative analysis of the structure and dynamics of wild-type transthyretin and its pathogenic variants: Insights from molecular dynamics simulations. 227th ACS national Meeting, Anaheim, CA, USA, American Chemistry Society
3. Shuanghong Huo, Mingfeng Yang, **Ming Lei** (2003). Molecular dynamics simulations of human transthyretin monomers. 17th Symposium of the Protein Society, Boston, MA, USA.
2. Mingfeng Yang, **Ming Lei**, Shuanghong Huo (2002). Molecular dynamics simulations on the wild-type human transthyretin and its variants. 224th ACS national Meeting, Boston, MA USA, American Chemistry Society.
1. **Lei Ming**, Feng Wenlin (1999). Ab initio MO Study on the Reaction Mechanism for Carbonyl Insertion. The 7th National Quantum Chemistry Conference, FuZhou, P. R. China, Chinese Chemical Society.