Curriculum Vitae of Ming Lei

ADDRESS

Ming Lei Ph.D
Professor
State Key Laboratory of Chemical Resource Engineering
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PERSONAL DATA

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

EMPLOYMENT HISTORY

Beijing University of Chemical Technology (BUCT):

Jan., 2015 – present	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

Feb. 2016 – March, 2016	Visiting Professor in Department of Chemistry in Princeton University (Princeton, NJ, USA).
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

Sept., 1990 – June, 1994	Beijing Normal University (Beijing, China), Advisor: Prof. Wenlin Feng B.S. in Chemistry in Hunan Normal University (Changsha City, Hunan Province)

PROFESSIONAL RESEARCH

Ming Lei has published 96 peer-review papers with H-index of 17.

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.

Biophysics and Computational Chemistry

Molecular dynamic simulation

Molecular modelling including molecular dynamics or Monte Carlo simulations to simulate dynamic features and compute thermodynamic and kinetic properties. Predicting three-dimensional structure of a protein from its amino acid sequence is a hot field in current structural biology. A lot of amyloid-related diseases are proposed to be related with protein folding and misfolding, such as Alzheimer's disease (AD), Huntington's disease (HD) and Parkinson's disease (PD). In the past 15 years, tremendous advances have been made with the development in experimental and theoretical technologies. Molecular dynamic (MD) simulation is one of the most realistic theoretical methods to predict native-like structures of peptides correctly. It could elucidate the folding features of small proteins at atom level. These dynamic features, which cannot be revealed by the X-ray crystallography, will provide significant insights into the origins of the qualitative differences in behavior and may also gain insight into what is likely to be the first step in the amyloid pathway.

Drug design

Besides crystallography, molecular modeling is of importance in structural biology and drug discovery. Using bioinformatic, docking and QSAR tools, we could make it clear on the binding modes of "keys" with the "lock". The three-dimensional shape of the lock based on experimental (X-ray or NMR structures) or theoretical methods (Homology models), it provides us a chance to design a lead compound to fit the lock precisely.

QM/MM study on transition metal biomolecular systems

Quantum mechanics with molecular mechanics (QM/MM) method is used to investigate biomolecular catalytic mechanisms.

PROFESSIONAL SKILLS

Quantum chemistry tools: Gaussian, QChem, Terachem, and so on,
Molecular simulation tools: 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

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)

Physical Chemistry (Undergraduate Students), 2000-2002, 2005-present (Fall & Spring)
Computational Catalysis (Graduate Students), 2019-present (Spring)
Chemoinformatics (Graduate Students), 2005-present (Fall)

REVIEW SERVICE TO PROFESSIONAL JOURNALS

Journal of the American Chemical Society
ACS Catalysis
ACS Applied Materials & Interfaces
Inorganic Chemistry
The Journal of Organic Chemistry
The Journal of Physical Chemistry
Organometallics
Langmuir
Industrial & Engineering Chemistry Research
ChemCatChem
Journal of Materials Chemistry A
Physical Chemistry Chemical Physics
Organic & Biomolecular Chemistry
Dalton Transaction
Catalysis Science and Technology
RSC Advance
European Journal of Inorganic Chemistry
Catalysis Letters
Catalysis Communications
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
Science China Chemistry
Acta Physico-Chimica Sinica
Chemical Journal of Chinese Universities
Sciencepaper Online
Chinese Journal of Structural Chemistry
CIESC Journal (Chemical Industry and Engineering Society of china)

GROUP MEMBERS:

GRADUATE STUDENTS

Yulan Dai	Ph.D Student (2019-present)	
Qaim Ali	Ph.D Student (2018-present)	
Wei Zhang	Ph.D Student (2016-present)	
Xingyu Chen	Ph.D Student (2015-present) with Assoc. Prof. Zhiqian Wang	
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)	Lecturer in China Univerersity of Mining & Technology, Biejing
Mawia H. Elsaim	Ph.D 2012 (2009-2012)	Lecturer in Sudan
Haohao Wang	2019-present	
Rui Wang	2019-present	
Chong Liu	2019-present	
Yaqi Zhao	2019-present with Prof. Min Pu	
Fuxing Shi	2019-present with Prof. Li Liu and Prof. Xiaolin Li	
Yuting Tao	2018-present with Assoc. Prof. Zuoyin Yang	
Xiaodi Zhang	2018-present	
Lin Zhang	2018-present	
Yangqiu Liu	2018-present	
Qianyue Wang	2017-present	
Ruiqing Ding	2017-present	
Chenguang Luo	2017-present	
Xin Yue	MA 2019 (2016-2019)	
Pengjie Li	MA 2019 (2016-2019)	
Yiwei Zhang	MA 2017 (2014-2017)	
Yanxia Xi	MA 2017 (2014-2017)	
Xinli Duan	MA 2016 (2013-2016)	
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
Houfang Wang	MA 2008 (2005-2008)	Staff in Tri-ibiotech Corp.

Yue Chen	MA 2009 (2006-2009)	Postdoc in Kyoto University

UNDERGRADUATE RESEARCH STUDENTS

Yinxing Zou	2019-present	
Zhewei Li	2018-present	
Ling Zhu	2019-present	
Xiaochuan Ren	2018-present	
Yunfeng Tu	2019-present	
Xiaoliang Liu	2018-present	
Fengze Han	2017-present	
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)	Postdoc in Tsinghua Univ.
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:

90. Zheliang Cao, Wei Zhang, Ruiqin Ding, Ju Wang, Min Pu, Zuoyin Yang, Ming Lei* (2019) “The reaction

paths of CH_2O decomposition on CuO(111) surface: a DFT study." J. Phys. Org. Chem.

89. Lin Zhang, Wei Zhang, Xin Yue, Pengjie Li, Zuoyin Yang, Min Pu, Ming Lei* (2019) "Theoretical Study on Mechanism of CO_2 Hydrogenation to Formic Acid Catalyzed by Manganese Complex." Chem. J. Chinese U. 40(9):1911-1917.
88. Yangqiu Liu, Xin Yue, Chenguang Luo, Lin Zhang, and Ming Lei* (2019) "Mechanisms of Ketone/Imine Hydrogenation Catalyzed by Transition-Metal Complexes." Energy Environ. Mater. DOI://10.1002/eem2.12050 (Review)
87. 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
86. 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 (Inside cover page)
85. 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, Back cover page)
84. Wei Zhang, Xuelu Ma, Hai Xiao, Ming Lei,* Jun Li* (2019) "Mechanistic Investigations on Thermal Hydrogenation of CO_2 to Methanol by Nanostructured CeO_2(100): The Crystal-Plane Effect on Catalytic Reactivity." J. Phys. Chem. C. 123 (18):11763–11771
83. 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
82. 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. 86:132-141
81. Jialuo She, Xiangfeng Lin, Zaihui Fu,* Jianwei Li,* Senpei Tang, Ming Lei, Xin Zhang, Chao Zhang, Dulin Yin (2019) "HCl and O_2 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
80. Jialing Ma, Hui Zhang, Xin Zhang,* **Ming Lei*** (2019) "3D-QSAR studies of D_3R antagonists and 5-$HT_{1A}R$ agonists." J. Mol. Graph. Model. 86:132-141
79. 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
78. 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
77. 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
76. 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
75. 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

74. 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
73. 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
72. Longfei Li, Huajie Zhu, Li Liu, Datong Song,* **Ming Lei*** (2018) "A Hydride-Shuttle Mechanism for the Catalytic Hydroboration of CO_2." Inorg Chem, 57: 3054−3060
71. 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
70. 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
69. 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 (PNAS), 114(37): 9803-9808
68. 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
67. 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
66. 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
65. 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
64. 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
63. 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
62. 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
61. Longfei Li, Yinna Bai, **Ming Lei**,* Li Liu* (2015) ”Progress in Rubber Vulcanization Accelerator.” Prog Chem 10:1500-1508 (Review in Chinese)
60. Xuelu Ma, **Ming Lei**,* Shubin Liu* (2015) ”Homolytic or Heterolytic Dihydrogen Splitting with Bimetallic Dinitrogen Complexes? A Computational Study.” Organometallics 34(7): 1255-1263
59. Xinli Duan, Min Zhang, Xin Zhang, Fang Wang*, **Ming Lei*** (2015) "Molecular Modeling and Docking Study on Dopamine D_2-likeand Serotonin $5HT_{2A}$ Receptors." J Mol Graph Model 57:143-155
58. **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
57. 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
56. Xuelu Ma, Yanhui Tang, **Ming Lei*** (2014) ”Bent and Planar Structures of μ-η^2, η^2-N_2 Dinuclear Early

Transition Metal Complexes." Dalton Trans 43 (30):11658-11666

55. **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
54. 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
53. 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
52. Lijun Zhao, **Ming Lei*** (2014) "Progress in computational chemical studies on transthyretin." Prog Chem 26(1):193-202 (Review, in Chinese)
51. Xuelu Ma, Yanhui Tang, **Ming Lei*** (2013) "Carboxylation of Hafnocene and Ansa-zirconocene Dinitrogen Complexes with CO_2: Insights from a DFT Study." Organometallics 32(23):7077-7082
50. 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):1083-1086
49. Xin Zhang, **Ming Lei*** (2013) "Which is the Proton-shuttle in Isoxanthopterin Deaminase? QM/MM MD Understanding." J Theor Comput Chem DOI: 10.1142/S0219633613410022
48. Lijun Zhao, Liangren Zhang*, **Ming Lei*** (2013). "A 3D-QSAR and Docking Study on Transthyretin Amyloidgenesis Inhibitors." Sci China Chem 56(11):1550-1563
47. Xuelu Ma, **Ming Lei*** (2013) "Progress in Dinitrogen Fixation Activated by Binuclear Transition-Metal Complexes." Prog Chem 25(8):1325-1333 (Review, in Chinese)
46. 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
45. 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
44. 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
43. Mawia Hassan, Xin Zhang*, Wenchao Zhang, Xiaojia Guo, Biaohua Chen, and **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
42. 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 14 (17), 6003 - 6012
41. 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
40. Wenchao Zhang, Yanhui Tang, **Ming Lei*,** Keiji Morokuma, Djamaladdin G. Musaev* (2011) "Ditantalum Dinitrogen complex: On reaction of H2 molecule 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):9481–949
39. 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
38. **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

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 Hydrogenation of ketones catalyzed by η6-Arene/N-Tosylethylenediamine-Ruthenium(II).” Organometallics 28(7):2078–2084
35. Yue Chen, Yanhui Tang,* **Ming Lei*** (2008). “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 (In press)
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 human transthyretin under partially denaturing conditions.” Biophysical J **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." J Struct Biol **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+CH_2O"." 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 $CH_2O+O[^3P]$ -> 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 SINICA **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). "CH_3NO_2+X(X = H, OH, CH_3, $CH_2[^3B_1]$,O[^{3}P])-> CH_2NO_2+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 $[CH_3ONO_2]H^+$ and R-OH." Journal of 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." Chemical Journal of Chinese Universities **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." The Journal of Chemical Physics **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 $RuH_2(CO)(PH_3)_3$." 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." Journal of 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." Chemical Research in Chinese University **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 Science 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." Journal of Chemical Physics **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 from1,2-Butadiene to 2-Butyne." Chemical Journal of Chinese Universities **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 Journal of Chemical Physics **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 Chemical Letters **8**: 71-72.
1. Hongxin Huang, Zexing Cao, **Ming Lei** (1996). "Self-optimizing diffusion quantum Monte Carlo calculation: the singlet-triplet splitting in CH_2." Journal of Molecular Structure (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.