

Curriculum Vitae of Ming Lei

ADDRESS

Ming Lei Ph.D
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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

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

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: 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)

AWARDS

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 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 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 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

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

REVIEW SERVICE TO PROFESSIONAL JOURNALS

Journal of the American Chemical Society
ACS Applied Materials & Interfaces
Inorganic Chemistry
Journal of Organic Chemistry
Organometallics
ChemCatChem
Physical Chemistry Chemical Physics
Organic & Biomolecular Chemistry
Catalysis Letters
Catalysis Communications
Journal of Molecular Catalysis B: Enzymatic
Journal of Physical Organic Chemistry
Chemical Biology & Drug Design
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
Chinese Journal of Structural Chemistry
CIESC Journal (Chemical Industry and Engineering Society of china)

GROUP MEMBERS:

GRADUATE STUDENTS

Hui Li	Ph.D student, 2014-present
Xuelu Ma	Ph.D student, 2010-present
Mawia H. Elsaim	Ph.D 2012 (2009-2012)
Yiwei Zhang	2014-present
Yanxia Xi	2014-present
Xinli Duan	2013-present
Zhidong Wang	2012-present
Yuhui Pan	2012-present
Min Zhao	MA 2013 (2011-2014)
Min Wang	MA 2013 (2011-2014)
Lijun Zhao	MA 2013 (2010-2013)
Ran Feng	MA 2013 (2010-2013)
Xiaojie Du	MA 2013 (2010-2013)
Qian Shen	MA 2012 (2010-2012)
Tianhu Yuan	MA 2012 (2009-2012)
Xiaojia Guo	MA 2012 (2009-2012)
Wenchao Zhang	MA 2011 (2008-2011)
Zhuo Chen	MA 2010 (2006-2010)
Baohua Zhang	MA 2010 (2006-2010)
Ang Xiao	MA 2010 (2006-2010)
Houfang Wang	MA 2008 (2005-2008)
Yue Chen	MA 2009 (2006-2009)

UNDERGRADUATE RESEARCH STUDENTS

Yiwei Zhang	B.S. 2014
Mo Zhang	B. S.2014
Yan Hu	B.S. 2010
Wenzheng Xie	B.S. 2010
Weiwei Xie	B.S. 2009
Lingzhou Zhao	B.S. 2009
Tianhu Yuan	B.S. 2009
Chunli Zhao	B.S. 2009
Yuanfu Yu	B.S. 2008
Yunhan Li	B.S. 2008

Zehan Hu	B.S. 2008 (2006-2008)
Hongbo Zhang	B.S. 2007
Hongjun Xie	B.S. 2006
Ruqiang Liu	B.S. 2006
Yue Chen	B.S. 2006

PUBLICATIONS:

59. Xinli Duan, Min Zhang, Xin Zhang, *Fang Wang,***Ming Lei** (2015) "Molecular Modeling and Docking Study on Dopamine D₂-like and 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 $\mu\text{-}\eta^2, \eta^2\text{-N}_2$ 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 CO₂: 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 12(8):1341002
48. Lijun Zhao, Liangren Zhang, **Ming Lei*** (2013). "A 3D-QSAR and Docking Study on Transthyretin Amyloidogenesis Inhibitors." Science 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, Djameladdin G. Musaev (2011) "Ditantalum Dinitrogen complex: On reaction of H₂ molecule with an "End-on-bridged" [TaV]₂(μ-η¹:η¹-N₂) and Bis(μ-nitrido) [TaV]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+CH₂O"." *Chinese Journal of Chemical Physics* **16**(2): 94-98.
 21. Yan Jianming, Lin Yuan, Wei Xianfu, Wang Yanqiao, Yang Lianming, **Lei Ming** (2002). "Evaluation 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 CH_x (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). "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." *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 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." *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 from 1,2-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 propyl nitrile." *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 CH₂." *Journal of Molecular Structure (Theochem)* **370**: 55-63.

CONFERENCES:

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 N₂ 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/CO₂ Assisted N₂ 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-metal 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 (WCCBMS 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 transthyretin **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.