Liangliang Huang
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EDUCATION

2012 Ph.D. Chemical Engineering, North Carolina State University, Raleigh, NC, U.S.A.
Thesis: "Computational Study of Toxic Gas Removal by Reactive Adsorption"
Advisor: Professor Keith E. Gubbins

2007 M.Sc. Chemical Engineering, Nanjing University of Technology, Nanjing, China.
Thesis: "The Investigation of Confined Fluids in Carbon Nanotubes by Computer Simulations"
Advisor: Professor Xiaohua Lu

2003 B.Sc. Chemical Engineering, Minor: Computer Science, Nanjing University of Technology, Nanjing, Jiangsu, China.

RESEARCH EXPERIENCE

2014.8 ~ Assistant Professor, University of Oklahoma, Norman, OK, U.S.A.

2014.1 ~ 2014.7 Research Associate, North Carolina State University, Raleigh, NC, U.S.A.

2012 - 2013 Postdoctoral Research Associate, North Carolina State University, Raleigh, NC, U.S.A.

2007 - 2012 Research Assistant, North Carolina State University, Raleigh, NC, U.S.A.

2003 - 2007 Research Assistant, Nanjing University of Technology, Nanjing, Jiangsu, China.

2003 Internship at the BASF-YPC Company Limited, Nanjing, Jiangsu, China.

Visiting Scientist:

2016 Adjunct Professor, Jiangxi Normal University, China
2014 Oak Ridge National Laboratory, Oak Ridge, U.S.A.
2013 Prof. Fernando Luis Barroso da Silva group, University of Sao Paulo at Ribeirao Preto, Brazil
Prof. Martin Schoen group, Technical University of Berlin, Berlin, Germany
Prof. Malgorzata Sliwinska-Bartkowiak group, Adam Mickiewicz University, Poznan, Poland

2012 Prof. Xiaohua Lu group, Nanjing University of Technology, Nanjing, Jiangsu, China.

2011 Prof. William A. Goddard III group, California Institute of Technology, Pasadena, California, U.S.A.
Prof. Adri van Duin group, Penn State University, University Park, Pennsylvania, U.S.A.

TEACHING EXPERIENCE

North Carolina State University (2007 ~ 2013)

CHE 315 Thermodynamics of Chemical and Phase Equilibria	2007, 2008, 2010 Spring
CHE 713 Advanced Thermodynamics	2008~2013 Fall
CHE 315 Chemical Process Thermodynamics	2009 Spring
CHE 775 Multi-Scale Modeling of Matter	2012 Fall, 2104 Spring
CHE 596 Chemical Principles of Engineering	2013 Spring

University of Oklahoma (2015 ~)

CHE 3313 Structure and Properties of Materials	2015, 2016, 2017 Spring
CHE 3474 Chemical Engineering Thermodynamics	2015, 2016 Fall
CHE 5480 Multi-Scale Modeling of Matter	2016 Spring

LEADERSHIP EXPERIENCE

March 3-5, 2010 Volunteer Team Leader, Summit Series on the National Academy of Engineering Grand Challenges, Raleigh, NC.

2009 - 2014.8 Coordinate seminars by overseas visitors and collaborators; Coordinate seminar series Molecular Theory and Simulation, attended by more than twenty theoretical research groups from North Carolina State University, Duke University and The University of North Carolina at Chapel Hill (http://gubbins.ncsu.edu/seminar.html).

2009 - 2014.8 Maintain group website and the group computer cluster; Coordinate the supercomputer allocations from National Science Foundation XSEDE program (https://www.xsede.org).

HONORS AND AWARDS

2016 ~ 2019 Adjunct Professor, Jiangxi Normal University, China, 2016-2019

2016 Presidential International Travel Fellowship (PITF), University of Oklahoma

2014 Research Excellence Award, State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing University of Technology, China, provided with a travel subsidy of $10,000 for four years.

2013 First Prize National Natural Science Award, Department of Education, China, the highest national award for natural science research, and the only first-prize project in Chemical Engineering, Project “Molecular thermodynamics and its applications in material-oriented chemical engineering”.

NSF Travel Award for “13th Properties and Phase Equilibria for Product and Process Design Conference (PPEPPD)”, Iguazu Falls, Argentina, May 26-30, 2013.

2012 Mentored Teaching Assistantship Award, College of Engineering, NC State University, providing outstanding graduate students with extensive teaching experience.

2011 Mentored Teaching Assistantship Award, College of Engineering, NC State University, providing outstanding graduate students with extensive teaching experience.

2010 NSF Travel Award for "12th Properties and Phase Equilibria for Product and Process Design Conference (PPEPPD)", Suzhou, Jiangsu, China, May 16-21, 2010.

2008 Second Prize State Science and Technology Advancement Award, Jiangsu, China, Project "Molecular modeling and thermodynamics research of material-oriented chemical engineering process".

2007 First Prize Shijun Research Award, Nanjing University of Technology, China, 2007, a university-wide annual award to five recipients.

PROFESSIONAL ASSOCIATIONS AND SERVICES

Membership: American Institute of Chemical Engineers, American Chemical Society

Referee: (19 journals) Langmuir, Industrial & Engineering Chemistry Research, Energy & Fuels, Molecular Simulation, Physical Chemistry Chemical Physics, Chemical Physics, Journal of Colloid and Surface Science, RSC Advance, Micromachines, Advance Science, Journal of Molecular Modeling, Journal of Physical Chemistry, Computational Materials Science, Chemical Communications, Journal of Materials Chemistry A, International Journal of Environmental Science and Technology, Journal of Chemical Physics, Journal of Chemical and Engineering Data, Chemical Engineering Science

REVIEW PANEL AND COMMITTEE

2014 ~ 2016	AIChE Area 1A Committee Member
2015	NSF GRFP Review Panel

ACADEMIC COMMITTEE

2014	Deepthi Konatham	Ph.D.	Advisor: Dr. Alberto Striolo
2015	Lauren Gilbert	M.Sc.	Advisor: Dr. Bin Wang
2016	Abby A. Baker	PhD.	Advisor: Dr. Bin Wang
2016	Alexander Kerr	PhD.	Advisor: Dr. Kieran Mullen
2016	Soumya Bhattacharya	Ph.D.	Advisor: Dr. Lloyd Bumm
2017	Tong Mou	Ph.D.	Advisor: Dr. Bin Wang
2017	Michael T. Warren	Ph.D.	Advisor: Dr. Jeffrey Harwell

STUDENTS

Undergraduate Researchers

Amy D. Do	Undergraduate Researcher	2014 - 2015
Isaree Darachai	Undergraduate Researcher	2015
Ke Jin	Undergraduate Researcher	2015
Andrew L. Rocha	Undergraduate Researcher	2015 - 2016
Garrett M. Tow	Undergraduate Research	2014 - 2015
Trevor R. Fisher	Undergraduate Research	2016 -
Robert J. Hill	Undergraduate Research	2017

Graduate Students

Sweta Surisetti	Master Student	2014 - 2015
Garrett M. Tow	Master Student	2015 - 2017
Guobing Zhou	PhD Student	2016 -
Qi Qiao	PhD Student	2016 -

Mohamed Z. Mehana PhD Student (Co-advise) 2016 -

Group Alumni

Garrett Tow Master May 2017 University of Notre Dame

VISTING SCHOLARS

Dr. Chang Liu	Associate Professor, Nanjing Tech University	2015 - 2016
Dr. Xiaobao Li	Associate Professor, Nanjing Forestry University	2015 - 2016
Dr. Zhen Yang	Professor, Jiangxi Normal University	2016 - 2017

PEER-REVIEW PUBLICATIONS

*** - Corresponding Author: 8;**
& - Undergraduate Student: 3;
Journal Cover: 1

40. Dongxue Li, Kiros Hagos, Liangliang Huang, Xiaohua Lu, Chang Liu and Hongliang Qian, "Self-Propagating High-Temperature Synthesis of Potassium Hexatitanate Whiskers", Ceramics International, 2017, accepted.

39. Yihui Dong, Rong An, Shuangliang Zhao, Wei Cao, Liangliang Huang, Wei Zhuang, Linghong Lu and Xiaohua Lu, "Molecular Interactions of Protein with TiO2 by AFM Measured Adhesion Force", Langmuir, 2017, accepted.

38. Lu Tan, Liangliang Huang, Qi Wang and Yingchun Liu, "A First Principles Study on O_2 Adsorption and Dissociation Processes over Rh(100) and Rh(111) Surfaces", Langmuir, 2017, accepted.

37. Li Li, Deshuai Yang, Trevor R. Fisher, Qi Qiao, Zhen Yang, Na Hu, Xiangshu Chen and Liangliang Huang, "Molecular Dynamics Simulations for Loading-Dependent Diffusion of CO_2, SO_2, CH_4, and Their Binary Mixtures in ZIF-10: The Role of Hydrogen Bond", Langmuir, 2017, accepted.

36. Rong An, Liangliang Huang, Kenneth P. Mineart, Yihui Dong, Richard J. Spontak and Keith E. Gubbins, "Adhesion and Friction in Polymer Films on Solid Substrates: Conformal Sites Analysis and Corresponding Surface Measurements", Soft Matter, 2017, 13, 3492-3505. (Back cover).

35. Wei Cao, Linghong Lu, Garrett M. Tow&, Liangliang Huang, Tingting Yang and Xiaohua Lu, "Hydrophilicity Effect on CO_2/CH_4 Separation using Carbon Nanotube Membranes: Insights from Molecular Simulation", Molecular Simulation, 2017, 43, 502-509.

34. Fu, Fangjia; Li, Yunzhi; Yang, Zhen; Zhou, Guobing; Huang, Yiping; Wan, Zheng; Chen, Xiang-Shu; Hu, Na; Li, Wei; Huang, Liangliang*, "Molecular-Level Insights Into Size-Dependent Stabilization Mechanism of Au Nanoparticles in 1-Butyl-3-Methylimidazolium Tetrafluoroborate Ionic Liquid", J. Pays. Chem. C, 2017, 121(1), 523-532.

33. Luchao Jin, Ahmad Jamili, Liangliang Huang and Felipe Perez, "Modeling the Mechanism of Clay Damage by Molecular Dynamics Simulation", Geofluids, 2017, 2017, 1747068.

32. Wei Cao, Linghong Lu, Liangliang Huang, Yihui Dong and Xiaohua Lu, "Molecular Behavior of Water on Titanium Dioxide Nanotubes: A Molecular Dynamics Simulation Study", J. Chem. Eng. Data, 2016, 61(12), 4131-4138.

31. Yaofeng Hu, Liangliang Huang, Shuangliang Zhao, Honglai Liu and Keith E. Gubbins, "Effects of Confinement in Nano-Porrous Materials on the Solubility of a Supercritical Gas", Molecular Physics, 2016, 114(22), 3294-3306.

30. Jing Zheng, Junqiao Zhang, Lu Tan, Debing Li, Liangliang Huang, Qi Wang and Yingchun Liu, "Effects of Aspect Ratio on Water Immersion into Deep Silica Nanoholes", Langmuir, 2016, 32(34), 8759-8766.

29. Wei Cao, Garrett M. Tow&, Linghong Lu, Liangliang Huang and Xiaohua Lu, "Diffusion of CO_2/CH_4 Confined in Narrow Carbon Nanotube Bundles", Molecular Physics, 2016, 114(16-17), 2530-2540.

28. Chang Liu, Yanhua Guo, Qiliang Hong, Chao Rao, Haijuan Zhang, Yihui Dong, Liangliang Huang*, Xiaohua Lu and Ningzhong Bao, "Bovine Serum Albumin Adsorption in Mesoporous Titanium Dioxide: Pore Size and Pore Chemistry Effect", Langmuir, 2016. 32(16), 3995-4003.

27. Xiaobao Li, Xue Zhang, Licheng Li, Liangliang Huang*, Wei Zhang, Judi Ye and Jianguo Hong, "Low-Temperature Hydrothermal Synthesis of ZnO/Regenerated Cellulose Nanocomposite", Materials Letters, 2016, 175, 122-125.

26. Guobing Zhou, Yunzhi Li, Zhen Yang, Fangjia Fu, Yiping Huang, Zheng Wan, Li Li, Xiangshu Chen, Na Hu and Liangliang Huang*, "Structural Properties and Vibrational Spectra of Ethylammonium Nitrate Ionic Liquid Confined in Single-Walled Carbon Nanotubes", J. Phys. Chem. C, 2016, 120(9), 5033-5041.

25. Rong An, Liangliang Huang, Yun Long, Berc Kalanyan, Xiaohua Lu and Keith E Gubbins, "Liquid-Solid Nano-friction and Interfacial Wetting", Langmuir, 2016, 32(3), 743-750.

24. Chang Liu, Jun Wang, Xiaoyan Ji, Liangliang Huang and Xiaohua Lu, "The Biomethane Producing Potential in China: A Theoretical and Practical Estimation", Chinese Journal of Chemical Engineering, 2016, 24(7), 920-928.

23. Xiaojing Guo, Guozhong Wu, Cheng Li, Hengfeng Gong, Jiangtao Hu, Chan Jin, Liangliang Huang* and Ping Huai, "DFT Investigations of Uranium Complexation with Amidoxime-, Carboxyl- and Mixed Amidoxime/Carboxyl-based Host Architectures for Sequestering Uranium from Seawater", Inorganica Chimica Acta., 2016, 441, 117-125.

22. Chang Liu, Nanhua Wu, Jun Wang, Liangliang Huang* and Xiaohua Lu, "Determination of the Ion Exchange Process of $K_2Ti_4O_9$ Fibers at Constant pH and Modeling with Statistical Rate Theory", RSC Adv., 2015, 5, 73474-73480.

21. Xiaojing Guo, Liangliang Huang, Cheng Li, Jiangtao Hu, Guozhong Wu and Ping Huai, "Sequestering Uranium from UO2(CO3)34- in Seawater with Amine Ligands: Density Functional Theory Calculations", Phys. Chem. Chem. Phys., 2015, 17, 14662-14673.

20. Liangliang Huang* and Keith E. Gubbins, "Ammonia Dissociation on Graphene Oxide: An ab initio Density Functional Theory Calculation", Z. Phys. Chem., 2015, 229, 1211-1223.

19. Liangliang Huang*, Keith E. Gubbins, Licheng Li and Xiaohua Lu, "Water on Titanium Dioxide Surface: A Revisit by Reactive Molecular Dynamics Simulations", Langmuir, 2014, 30, 14832.

18. Long Chen, Liangliang Huang, and Jiahua Zhu, "Stitch Graphene Oxide Sheets into Membrane at Liquid/Liquid Interface", Chem. Commun., 2014, 50, 15944.

(1-17 are before OU)

17. Wei Cao, Linghong Lu, Liangliang Huang, Shanshan Wang, and Yudan Zhu, "Molecular Simulations on Diameter Effect of Carbon Nanotube for Separation of CO_2/CH_4", CIESC J., 2014, 65, 1736.

16. Liangliang Huang, Mykola Seredych, Teresa J. Bandosz, Adri C. T. van Duin, Xiaohua Lu and Keith E. Gubbins, "Controllable Atomistic Graphene Oxide Model and its Application in Hydrogen Sulfide Removal", J. Chem. Phys., 2013, 139, 194707.

15. Liangliang Huang, Teresa J. Bandosz, Kaushik L. Joshi, Adri C. T. van Duin, and Keith E. Gubbins, "Reactive Adsorption of Ammonia and Ammonia/Water on CuBTC Metal-Organic Framework: a ReaxFF Molecular Dynamics Simulation", J. Chem. Phys., 2013, 138, 034102.

14. Liangliang Huang, Kaushik L. Joshi, Adri C. T. van Duin, Teresa J. Bandosz, and Keith E. Gubbins, "ReaxFF Molecular Dynamics Simulation of Thermal Stability of a $Cu_3(BTC)_2$ Metal-Organic Framework", Phys. Chem. Chem. Phys., 2012, 14, 11327.

13. Camille Petit, Liangliang Huang, Jacek Jagiello, Jeffrey Kenvin, Keith E. Gubbins, and Teresa J. Bandosz, "Towards Understanding Reactive Adsorption of Ammonia on Cu-MOF/Graphite Oxide Nanocomposites", Langmuir, 2011, 27, 13043.

12. M. Jazdzewska, M. Sliwinska-Bartkowiak, Anatoly Beskrovny, Sergey G. Vasiloskly, Siu-Wa Ting, Kwong-Yu Chan, Liangliang Huang, and Keith. E. Gubbins, "Novel Ice Structures in Carbon Nanopores: Pressure Enhancement Effect of Confinement", Phys. Chem. Chem. Phys., 2011, 13, 9008.

11. M. Sliwinska-Bartkowiak, M. Jazdzewska, Keith E. Gubbins and Liangliang Huang, "Melting Behavior of Bromobenzene within Carbon Nanotubes", J. Chem. Eng. Data, 2010, 55, 4183.

10. M. Sliwinska-Bartkowiak, M. Jazdzewska, Liangliang Huang and Keith E. Gubbins, "Melting Behavior of Water in Cylindrical Pores: Carbon Nanotubes and Silica Glasses", Phys. Chem. Chem. Phys., 2008, 10, 4909.

9. Qing Shao, Liangliang Huang, Jian Zhou, Linghong Lu, Luzheng Zhang, Xiaohua Lu, Shaoyi Jiang, Keith E. Gubbins, and Wenfeng Shen, "Molecular simulation study of temperature effect on ionic hydration in carbon nanotubes", Phys. Chem. Chem. Phys., 2008, 10,1896.

8. Qing Shao, Liangliang Huang, Xiaohua Lu, Linghong Lu, Yudan Zhu, and Wenfeng Shen, "Molecular simulation study of the structure and diffusion of ethanol molecules confined in carbon nanotubes", Acta. Chimica. Sinica., 2007, 65, 2217.

7. Linghong Lu, Qing Shao, Liangliang Huang and Xiaohua Lu, "Simulation of adsorption and separation of ethanol–water mixture with zeolite and carbon nanotube", Fluid Phase Equilibria, 2007, 261, 191.

6. Qing Shao, Liangliang Huang, Jan Zhou, Linghong Lu, Luzheng Zhang, Xiaohua Lu, Shaoyi Jiang, Keith E. Gubbins, Yudan Zhu and Wenfeng Shen, "Molecular dynamics study on diameter effect in structure of ethanol molecules confined in single-walled carbon nanotubes", J. Phys. Chem. C, 2007, 111, 15677.

5. Linghong Lu, Xiaohua Lu, Yuping Chen, Liangliang Huang, Qing Shao and Qi Wang, "Monte Carlo simulation of adsorption of binary and quaternary alkane isomers mixtures in zeolites: Effect of pore size and structure", Fluid Phase Equilibria, 2007, 259, 135.

4. Yuping Chen, Linghong Lu, Qing Shao, Liangliang Huang, and Xiaohua Lu, "Adsorption and Diffusion of Alkanes in Mordenite", Acta Physico-Chimica Sinica, 2007, 23, 905.

3. Liangliang Huang, Luzheng Zhang, Qing Shao, Jun Wang, Linghong Lu, Xiaohua Lu, Shaoyi Jiang, and Wenfeng Shen, "Simulations of Binary Mixture Adsorption of Carbon Dioxide and Methane in Carbon Nanotubes: Temperature, Pressure, and Pore Size Effects", J. Phys. Chem. C, 2007, 111, 11912.

2. Liangliang Huang, Luzheng Zhang, Qing Shao, Jun Wang, Linghong Lu, Xiaohua Lu, Shaoyi Jiang, and Wenfeng Shen, "Molecular Dynamics Simulation Study of the Structural Characteristics of Water Molecules Confined in Functionalized Carbon Nanotubes", J. Phys. Chem. B, 2006, 110, 25761.

1. Liangliang Huang, Qing Shao, Linghong Lu, Xiaohua Lu, Luzheng Zhang, Jun Wang, and Shaoyi Jiang, "Helicity and Temperature Effects on Static Properties of Water Molecules Confined in Modified Carbon Nanotubes", Phys. Chem. Chem. Phys., 2006, 8, 3836.

CONFERENCE ORAL PRESENTATIONS

1. "Simulations of Binary Mixture Adsorption of Carbon Dioxide and Methane in Carbon Nanotubes", AIChE Annual Meeting, San Francisco, CA, USA, November 12 - 17, 2006.

2. "Density Functional Theory Study of the Adsorption and Reaction of Toxic Gases on Carbon Materials", IGRTG 1524, 1st Annual Meeting, Dollnsee, Germany, July 27, 2010.

3. "Ammonia Dissociation over Graphite Oxide, Carbon Nanotubes and Fullerene", AIChE Annual Meeting, Salt Lake City, UT, USA, November 8 - 12, 2010.

4. "A Reactive Molecular Dynamics Simulation of Hydrogen Sulfide Dissociation over Graphene Oxide", IGRTG 1524, 2nd Annual Meeting, New Bern, Raleigh, NC, USA, October 3 - 6, 2011.

5. "Ammonia Adsorption on Cu-MOF: a Molecular Simulation Approach", AIChE Annual Meeting, Minneapolis, MN, USA, October 17 - 21, 2011.

6. "A Reactive Molecular Dynamics Simulation of Hydrogen Sulfide Dissociation over Graphene Oxide", AIChE Annual Meeting, Minneapolis, MN, USA, October 17 - 21, 2011.

7. "Surface Chemistry of TiO_2: Hydrophilic or Hydrophobic", AIChE Annual Meeting, Pittsburgh, PA, USA, October 28 - November 2, 2012.

8. "Reactive Molecular Dynamics Simulation of Graphite Oxide and Its Application in Hydrogen Sulfide Removal", FOA11, 11th International Conference on the Fundamentals of Adsorption, Baltimore, MD, USA, May 19 - 24, 2013.

9. "Choline Chloride / Urea and its Application towards CO_2 Capture and Storage", IGRTG 1524, 3rd Annual Meeting, New Bern, NC, USA, September 29 - October 3, 2013.

10. "Controllable Phase Transition of CuBTC Metal-Organic Framework and Its Application in CO_2 Capture and Storage", AIChE Annual Meeting, San Francisco, CA, USA, November 3 - 8, 2013.

11. "A Theoretical Understanding of Amino Acid Interaction with Graphene and Its Derivatives", AIChE Annual Meeting, Atlanta, GA, USA, November 16-21, 2014.

12. "The Role of Polymer-Substrate Interaction Strength in Polymer Films on Solid Substrates: Friction Force and the Glass Transition", AIChE Annual Meeting, Salt Lake City, UT, USA, November 8-13, 2015.

13. "Amino Acid Adsorption on Graphene Oxide, Titanium Dioxide and Their Composites",14th Properties and Phase Equilibria for Product and Process Design (PPEPPD), Porto, Portugal, May 22 - 26, 2016.

14. "Amino Acid Adsorption on Graphene Oxide and Titanium Dioxide", The 4th International Conferences on Sustainable Chemical Product and Process Engineering, SCPPE2016, Nanjing, China, May 31 - June 3, 2016.

15. "Amino Acid Adsorption on Titanium Dioxide Surface: A Reactive Molecular Dynamics Simulation", AIChE Annual Meeting, San Francisco, CA, USA, November 13-18, 2016.

CONFERENCE POSTER PRESENTATIONS

1. "Temperature and Pressure Effects on Hydrogen Bonds of Supercritical Water Confined in Carbon Nanotube: A Molecular Dynamics Study", AIChE Annual Meeting, San Francisco, CA, USA, November 12 - 17, 2006.

2. "Phase Transitions of Liquids in Carbon Nanotubes: STM Characterization of Carbon Nanotube", US-Poland Workshop, Gdansk, Poland, June 2-7, 2008.

3. "Freezing/Melting of Liquids in Cylindrical Nanopores", Characterization of Porous Solids 8, Edinburgh, Scotland, June 10 - 13, 2008.

4. "Effect of Wall-Water Interaction on Filling and Structure of Water inside Nanotube", AIChE Annual Meeting, Philadelphia, PA, USA, November 15 - 21, 2008.

5. "Freezing/Melting of Liquids in Cylindrical Nanopores", AIChE Annual Meeting, Philadelphia, PA, USA, November 15 - 21, 2008.

6. "DFT Study of Dissociative Adsorption of H_2S on Defective Carbon Subtracts",12th Properties and Phase Equilibria for Product and Process Design (PPEPPD), Suzhou, China, May 16 - 21, 2010.

7. "Reactive Adsorption of Ammonia on CuBTC Metal-Organic Framework: a ReaxFF Molecular Dynamics Simulation", 6th International Workshop on Characterization of Porous Materials: from Angstroms to Millimeters (CPM-6), Delray Beach, Florida, USA, April 30 - May 2, 2012.

8. "CuBTC Metal-Organic Framework: Thermal Stability, Hydrostatic Stability and Reactive Adsorption of Ammonia", FOMMS 2012 Foundations for Discovery and Data, Portland, Oregon, USA, July 22 - 26, 2012.

9. "The Design of Titanium Dioxide Surface Chemistry by Molecular Modeling", 13th Properties and Phase Equilibria for Product and Process Design (PPEPPD)", Iguazu Falls, Argentina, May 26 - 30, 2013.

10. "Interactions between Amino Acid and Graphene Oxide: Experiments and Theoretical Calculations", ACS Annual Meeting, Denver, CO, USA, March 22-26, 2015.

11. "How Surface Chemistry Affects Amino Acids Adsorption on Graphene-based Materials?", The 7th International Workshop Characterization of Porous Materials: from Angstroms to Millimeters (CPM-7), Delray Beach, Florida, USA, May 3-6, 2015.

12. "Molecular Dynamics Simulation of C_{60}/Graphite/Water Systems: Dry and Wet Surface Friction", FOMMS 2015 Foundations for Discovery and Data, Portland, Oregon, USA, July 12 - 16, 2015.

INVITED: TALK, SEMINAR, WORKSHOP AND COURSE

1. "NH_3 Removal by Adsorptive Reaction", Materials and Process Simulation Center, California Institute of Technology, Pasadena, CA, USA, January 5, 2011.

2. "Chemisorption and Chemical Reaction: Reactive Molecular Dynamics Simulation & *ab initio* DFT Method", The Babcock & Wilcox Company, Akron, OH, November 12, 2012.

3. "Reactive Molecular Dynamics Simulation of H_2O/TiO_2 Interactions", Nanjing University of Technology, Nanjing, Jiangsu, China, December 1, 2012.

4. "Computational Study of Toxic Gas Removal by Reactive Adsorption", Nanjing University of Technology, Nanjing, Jiangsu, China, December 7, 2012.

5. "Multi-Scale Modeling of Matter: a short Introduction from Algorithm to Application", Nanjing University of Technology, Nanjing, Jiangsu, China, December 8-10, 2012 (workshop).

6. "Reactive Molecular Dynamics Simulation of Graphene Oxide and its Application in Hydrogen Sulfide Removal", Workshop on Molecular Interactions and Nanobiological Applications, University of São Paulo, Ribeirão Preto, Brazil, June 25 - 26, 2013 (workshop).

7. "Confined Fluids in Carbon Nanotubes: a Case Study by Molecular Modeling", "*Ab initio* DFT and Reactive Molecular Dynamics Simulation: a Case Study of Graphene Oxide", Symposium on Nanostrcuture and Nanophases, Adam Mickiewicz University, Poznan, Poland, July 17, 2013. (workshop)

8. "Choline Chloride / Urea and its Application towards CO_2 Capture and Storage", Department of Chemistry, Technical University of Berlin, Berlin, Germany, July 26, 2013.

9. "Computational Chemistry, A Short Course", Zhejiang University, China, July 18-26, 2016.

10. "A Theoretical Understanding of Amino Acid Interaction with Graphene and its Derivatives", The International WorkShop on "Advances in the Studies of Mesoscale problems", Shanghai, China, September 22-26, 2016.

11. "Reactive Molecular Dynamics Simulation and Its Applications: An Introduction and Examples", Institute of Applied Physics, Chinese Academy of Science, China. September 28, 2016.

12."A Theoretical Understanding of Amino Acid Interaction with Graphene and Its Derivatives", The 9th International Conferences on Computational Nanoscience and New Energy Materials, CNNEM2016, Shanghai, China, June 22 - 26, 2016.

13. "Amino Acid Adsorption on Graphene Oxide, Titanium Dioxide and their Composites", Materials Science & Technology 16, Salt Lake City, UT, October 23-27, 2016.

14. "Amino Acid Adsorption on Titanium Dioxide Surface: A Reactive Molecular Dynamics Simulation", Jiangxi Normal University of Technology, China, May 19, 2017.

15. "H_2S and Gas-Field Corrosion: Mechanism, Computation and Evaluation", Natural Gas Research Institute, Southeast Oil Field, PetroChina, China, May 25, 2017.

16. "Modeling of Graphene Oxide", Nanjing University of Technology, China, May 30, 2017.

17. "Theory and Modeling of Graphene Oxide and Its Derivatives", 2017 International Workshop on Advance Materials and Interfacial Thermodynamics, Jiangnan Graphene Research Institute, Changzhou, China, June 1-2, 2017.

18. "Some Thoughts of Carbon Materials and Their Modeling", Nanjing University of Science and Technology, China, June 5, 2017.

19. "The TiO_2/H_2O System: Possible Water Induced Hydrophobicity?", International Workshop on Mesoscale Theory and Simulation for Interfacial Problems, East China University of Science and Technology, China, June 9-10, 2017.

20. "Amino Acid Adsorption on Titanium Dioxide Surface: A Reactive Molecular Dynamics Simulation", Zhejiang University of Technology, China, June 19, 2017.

Service

University of Oklahoma

2016- AIChE Student Chapter Advisor

2016- Core member in promoting department level collaborations with two Chinese universi ties: Nanjing Tech University, East China University of Science and Technology, China

Professional Memberships and Service

2014- 2017 Area 1A Committee Member, AIChE

2016 Regional Member, 76th Physical Electronics Conference, June 20-23, 2016, Fayetteville, AR, USA.

Meeting and Symposium Organizer

Chair, "Symposium on Molecular Theory and Modeling: In Honor of the 80th Birthday of Professor Keith E. Gubbins", NC State University, Raleigh, NC, May 1, 2017

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