

# 个人简历

## 个人信息

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## 教育背景

2000年9月至2004年7月 华东师范大学物理系 物理学学士  
2004年9月至2010年6月 华东师范大学物理系 凝聚态物理学博士  
2008年1月至2009年1月 美国加州大学戴维斯分校材料科学与工程系 国家公派联合培养博士生

## 工作/科研经历

2014年9月至今 华东师范大学物理学系 紫江青年学者特聘研究员

2013年8月至2014年8月 美国加州大学伯克利分校材料科学与工程系 材料科学博士后

在Mark Asta教授课题组从事电解液/电极界面(新能源存储相关的超级电容器与锂电池)的计算模拟研究。研究经费由美国能源部能源前沿研究中心(Energy Frontier Research Centers) DE-SC0001342号合同提供。

2011年1月至2013年8月 美国堪萨斯大学化学系 理论物理化学博士后

在Brian Laird教授课题组从事异质固液界面和液液界面的热力学与结构基础理论研究。研究经费由美国国家科学基金会(National Science Foundation) CHE0957102号合同提供。

2010年8月至2011年1月 复旦大学物理系 科研助理

在龚新高教授课题组从事热能存储相变材料的相关基础研究,研究涉及纳米颗粒的熔点与熔化潜热的理论计算。

2008年1月至2009年1月 美国加州大学戴维斯分校材料科学与工程系 联合培养材料科学博士生

师从Mark Asta教授进行合金快速凝固过程的计算模拟研究。研究经费由美国能源部基础能源科学办公室DE-FG02-06ER46282号合同提供。

2004年7月至2010年7月 华东师范大学物理学系 凝聚态物理博士生

师从孙得彦教授进行纳米尺度材料和结构和稳定性的理论研究。

## 科学学会会员

- ◇ 美国物理学会会员(American Physical Society)
- ◇ 英国皇家化学学会会员(The Royal Society of Chemistry)

## 学术兼职

- ◇ 专业期刊Computational Material Science审稿人
- ◇ 专业期刊Rare Metals审稿人

## 奖励荣誉

- ◇ 国家留学基金委国家建设高水平大学公派研究生奖学金 2008年
- ◇ 博士论文入选上海市研究生优秀成果（学位论文） 2011年
- ◇ 入选参加美国能源部能源前沿研究中心于橡树岭国家实验室举办的关于结构材料核辐射损伤、缺陷、形变的暑期学校 2012年
- ◇ 获加州大学洛杉矶分校理论数学和应用数学中心资助，参加材料缺陷的原子与介观尺度模拟研讨会 2012年

## 教学活动

- ◇ 2016年秋季学期：高等固体物理（研究生必修课程）
- ◇ 2016年秋季学期：华东师范大学菁英班导师

## 研究方向

关键词：Molecular Dynamics Simulation Algorithms; Solid-Liquid Interfaces(SLIs); Electrode-Electrolyte Interfaces; Thermodynamics and Kinetics of SLIs; Interfacial Phase Diagram; Interfacial Phase Transition; Properties of Glasses and Supercooled Liquids; Inhomogeneous Fluids; Liquid-State Theory; Confined Water; Computational Condensed Matter Physics, Material Science and Physical Chemistry.

本人研究涉及物质界面体系基础物理学理论，以及能源和环境物理的核心问题。研究集中在下列三个主要方向：（一）块体材料（固相-液相-汽相）和其界面的结构、热力学和动力学理论。（二）纳米材料的热力学和结构相图；纳米液滴的动态湿润和铺展动力学；纳米尺度的弹性毛细现象。（三）发展模拟电极/电解液界面的分子动力学方法；研究相关的界面结构、热力学、电化学和动电性质，在分子尺度下拓展传统电双层结构连续介质理论模型；研究提高锂电池和超级电容的性能的核心界面参数和性质。研究将结合分子模拟技术和先进界面结构表征技术开展，同时比较上述研究领域的已有理论模型并发

展建立新理论。

## 主持经费

- ◇ 紫江青年学者启动经费，100万，2014年9月-2019年7月，项目负责人
- ◇ 中国自然科学基金青年项目“异质固-液界面自由能的计算研究”，24万，2016年9月-2018年12月，项目负责人

## 主要成果

- ★ 设计高精度的原子模拟实验，揭示了金属铅液滴在金属铝固体中的布朗运动这个奇异现象的物理机制。本研究与世界顶级透射电子显微镜研究团队(劳伦斯伯克利国家实验室国家电子显微术中心主任Uli Dahmen的研究团队)合作进行。研究论文正在准备中。
- ★ 首次预言自然界中存在第三类界面预融化相变发生在异质固液界面中，前两类为固体表面预融化相变和晶界预融化相变。研究成果已在物理专业顶级期刊Physical Review Letters上以第一作者公开发表(Phys. Rev. Lett. 110, 096102, 2013)。
- ★ 创立了一套崭新的方法来表征合金固液界面体系的非平衡态性质和计算合金界面的动力学性质，并达到空前的统计精度。通过使用这套方法：我们首次定量测量了合金固液界面对溶质原子的俘获效应和其各向异性；首次直接观测到合金体系快速凝固过程中溶质俘获的突变现象，澄清了各种唯象模型间的长期争论；首次定量分析了合金界面的溶质阻滞效应，计算出合金固化过程中固液界面的迁移率和其各向异性；首次发现了固液界面动力学模拟中的温度梯度，从而正确地计算了非平衡相变过程中的热力学驱动力。以上新方法和重要发现为合金界面动力学理论的发展开辟了新的机遇，并在物理专业顶级期刊Physical Review Letters上以第一作者公开发表(Phys. Rev. Lett. 107, 25505, 2011)。
- ★ [Phys. Rev. Lett. 107, 25505, 2011]整篇文章被收录为[“Solidification of Containerless Undercooled Melts” Editors: D. M. Herlach and D. M. Matson, 2012, Wiley-VCH Verlag & Co. KGaA, Boschstr. 12, 69469, Weinheim, Germany]书中第17章。
- ★ 发表文章“Determination of the Crystal-Melt Interface Kinetic Coefficient from Molecular Dynamics Simulations”荣获Modelling Simul. Mater. Sci. Eng.期刊2010年亮点文章第一名，该年共10篇文章入选。共被下载2160次。
- ★ 建立了毛细作用驱使的弹性管形变的理论模型，并首次预言该体系存在新的弹性毛细普适标度关系；我们首次使用计算机模拟的方法研究弹性毛细现象，并通过对有液体填充的碳纳米管进行分子动力学模拟验证了我们理论所预言的普适标度关系。以上研究成果已在物理专业一流期刊Physical Review B Rapid Communications上以第一作者公开发表。
- ★ 发表文章“Evaluation of Constant Potential Method in Simulating Electric Double-Layer Capacitors”荣获J. Chem. Phys.第141卷18期封面文章和Featured article。

## 发表论文

(所列19篇论文, SCI收录16篇。至2016年3月22日, 被引用153次, H因子8)

1. **Y. Yang**, H. Humadi, D. Buta, B. B. Laird, D. Y. Sun, J. J. Hoyt and M. Asta, "Atomistic Simulations of Nonequilibrium Crystal-Growth Kinetics from Alloy Melts", *Phys. Rev. Lett.*, 107, 025505, (2011). [影响因子7.943] [已被引用34次]  
◇ [Phys. Rev. Lett. 107, 25505, 2011]整篇文章被收录为["Solidification of Containerless Undercooled Melts" Editors: D. M. Herlach and D. M. Matson, 2012, Wiley-VCH Verlag & Co. KGaA, Boschstr. 12, 69469, Weinheim, Germany]书中第17章。
2. **Y. Yang**, M. Asta and B. B. Laird, "Solid-Liquid Interfacial Premelting", *Phys. Rev. Lett.*, 110, 096102, (2013). [影响因子7.943] [已被引用4次]
3. **Y. Yang**, D. L. Olmsted, M. Asta and B. B. Laird, "Atomistic Characterization of the Chemically Heterogeneous Al-Pb Solid-Liquid Interface", *Acta Mater.*, 60, 4960, (2012). [影响因子3.941] [已被引用12次]
4. **Y. Yang**, Y. F. Gao, D. Y. Sun, M. Asta and J. J. Hoyt, "Capillary Force-induced Structural Deformation in Liquid Infiltrated Elastic Circular Tubes", *Phys. Rev. B: Rapid Communications*, 81, 241407, (2010). [影响因子3.767] [已被引用13次]
5. **Y. Yang** and B. B. Laird, "Atomistic Simulation Study of Capillary Fluctuation, Interfacial Free Energy and Structure of Al-Pb Liquid-Liquid Interface", *J. Phys. Chem. B*, 118, 8373, (2014). [影响因子3.607]  
◇ 专刊约稿。
6. **Y. Yang**, D. Y. Sun and X. G. Gong, "Prediction of Structural Evolution for Clusters: The Pair Potential Cases", *Chem. Phys. Lett.*, 474, 119, (2009). [影响因子2.145]
7. **Y. Yang** and D. Y. Sun, "Effect of the Equilibrium Pair Separation on Cluster Structures", *Commun. Comput. Phys.*, 6, 730, (2009). [影响因子1.863] [已被引用1次]
8. Q. Shu, **Y. Yang**, Y. T. Zhai, D. Y. Sun, H. J. Xiang and X. G. Gong, "Size-dependent Melting Behavior of Iron Nanoparticles by Replica Exchange Molecular Dynamics", *Nanoscale*, 4, 6307, (2012). [影响因子6.233] [已被引用13次]
9. W. Q. Wu, **Y. Yang**, Q. H. Yuan and D. Y. Sun, "The Collapse of an Elastic Tube Induced by Encapsulated Liquid Droplets", *Soft Matter*, 9, 9774, (2013). [影响因子3.909]
10. B. B. Laird, R. L. Davidchack, **Y. Yang** and M. Asta, "Determination of the Solid-Liquid Interfacial Free Energy Along a Coexistence Line by Gibbs-Cahn Integration", *J. Chem. Phys.*, 131, 114110, (2009). [影响因子3.164] [已被引用22次]
11. Z. X. Wang, **Y. Yang**, D. L. Olmsted, M. Asta and B. B. Laird, "Evaluation of Constant Potential Method in Simulating Electric Double-Layer Capacitors", *J. Chem. Phys.*, 141, 184102, (2014). [影响因子3.164] [已被引用6次]  
◇ 荣获J. Chem. Phys.第141卷18期封面文章和Featured article。收录为该期刊的2014 Editors' Choice Collection。
12. J. Monk, **Y. Yang**, M. I. Mendeleev, M. Asta, J. J. Hoyt and D. Y. Sun, "Determination of the Crystal-Melt Interface Kinetic Coefficient from Molecular Dynamics Simulations", *Modelling Simul. Mater. Sci. Eng.*, 18, 015004, (2010). [影响因子1.932] [已被引用26次]  
◇ 荣获Modelling Simul. Mater. Sci. Eng.期刊2010年亮点文章第一名, 该年共10篇文章入选。
13. X. Q. Zheng, **Y. Yang**, Y. F. Gao, J. J. Hoyt, M. Asta and D. Y. Sun, "Disorder Trapping During Crystallization of the B2 Ordered NiAl System", *Phys. Rev. E*, 85, 041601, (2012). [影响因子2.313] [已被引用10次]
14. Y. F. Gao, **Y. Yang**, D. Y. Sun, M. Asta and J. J. Hoyt, "Molecular Dynamics Simulations of the Crystal-Melt Interface Mobility in HCP Mg and BCC Fe", *J. Cryst. Growth*, 312, 3238, (2010). [影响因子1.552] [已被引用10次]

15. Y. F. Gao, **Y. Yang** and D. Y. Sun, “A Comparing Study of the Wetting Behavior of Iron Droplet in Carbon Nanotube and on Graphene Sheet”, *Chin. Phys. Lett.*, 28, 4, (2011). [影响因子1.078] [已被引用2次]
16. X. Q. Zheng, **Y. Yang**, D. Y. Sun, “Atomistic Characterization of a Modeled Binary Ordered Alloy Solid-Liquid Interface”, *Acta Phys. Sin.*, 62, 17101, (2013). [影响因子1.027]
17. B. B. Laird, R. L. Davidchack, **Y. Yang** and M. Asta, “Calculation of Solid-Liquid Interfacial Free Energies from Atomistic Computer Simulation”, *Proceedings of the Fifth International Conference Multiscale Materials Modeling*, 464, (2010).
18. H. Humadi, **Y. Yang**, D. Buta, B. B. Laird, D. Y. Sun, J. Hoyt, M. Asta, “Direct Computation of the Solute Drag on a Moving Interface using Atomistic Simulations”, *AIP Conference Proceedings*, (2012).
19. H. Y. Zhang, F. Liu, **Y. Yang**, W. X. Hu and D. Y. Sun, “Non-equilibrium Molecular Dynamics Study on the Defect Trapping during Solidification of Ni and Al”, *J. Chem. Phys.*, *Submitted*, (2016).

## 会议报告

1. The Fall Chinese Physical Society Meeting, Beijing, China, September, 2006; “The Classification of Cluster Structure.” **Y. Yang** and D. Y. Sun. (口头报告*Oral Presentation*)
2. The Fall Chinese Physical Society Meeting, Beijing, China, September, 2006; “The Evolution of Cluster Structures with a Model Potential.” **Y. Yang** and D. Y. Sun. (口头报告*Oral Presentation*)
3. Physical Chemistry Seminar, Department of Chemistry, University of Kansas, Lawrence, Kansas, United States, February, 2011; “Rapid Solidification of Lennard-Jones Binary Alloy.” **Y. Yang**, H. Humadi, D. Buta, D. Y. Sun, J. Hoyt, B. B. Laird and M. Asta. (邀请报告*Invited Talk*)
4. Kansas Physical Chemistry Symposium, Manhattan, Kansas, United States, October, 2011; “Interfacial Structure and Wetting of Liquid Lead on Aluminum.” **Y. Yang**, D. L. Olmsted, M. Asta and B. B. Laird. (海报展示*Poster Presentation*)
5. Physical Chemistry Seminar, Department of Chemistry, University of Kansas, Lawrence, Kansas, United States, November, 2011; “Interfacial Structure and Wetting of Liquid Lead on Aluminum.” **Y. Yang**, D. L. Olmsted, M. Asta and B. B. Laird. (邀请报告*Invited Talk*)
6. Kansas Physical Chemistry Symposium, Manhattan, Kansas, United States, October, 2012; “Roughening and Premelting at the Al/Pb Solid-Liquid Interface: a Molecular- Dynamics Simulation Study.” **Y. Yang**, M. Asta and B. B. Laird. (口头报告*Oral Presentation*)
7. Workshop on Atomistic and Mesoscale Modeling of Material Defects, Institute for Pure and Applied Mathematics (IPAM), University of California, Los Angeles, California, United States, October, 2012; “Calculation of Interfacial Free Energy for Chemically Heterogeneous Liquid-Liquid Interface.” **Y. Yang**, M. Asta and B. B. Laird. (海报展示*Poster Presentation*)
8. M2F2 Seminar, Department of Aerospace Engineering, University of Kansas, Lawrence, Kansas, United States, April, 2013; “Solid-Liquid Interfacial Premelting and Related Wetting/Spreading Phenomenon.” **Y. Yang**, M. Asta and B. B. Laird. (邀请报告*Invited Talk*)
9. Department Seminar, Department of Physics, Donghua University, Shanghai, China, May, 2014; “Atomistic Simulation Study of Heterogeneous Solid-Liquid Interface.” **Y. Yang**, M. Asta and B. B. Laird. (邀请报告*Invited Talk*)
10. Faraday Discussion 176: Next-Generation Materials for Energy Chemistry, Xiamen, China, October, 2014; “Molecular Dynamics Study of Ion Diffusion Barrier at Electrolyte/Electrode Interface.” **Y. Yang**, Z. X. Wang, D. L. Olmsted, B. B. Laird and M. Asta. (海报展示*Poster Presentation*)

11. CMRS2015 Annual Meeting and Exhibition, Guiyang, China, July 11, 2015; “Solid-Liquid Interfacial Premelting and its Applications: in Brownian Motion of Liquid Inclusions, Wetting/Spreading.” **Y. Yang**, B. B. Laird and M. Asta. (邀请报告 *Invited Talk*)
12. CMRS2015 Annual Meeting and Exhibition, Guiyang, China, July 11, 2015; “Thermodynamics and Intrinsic Structure of the Al-Pb Liquid/Liquid Interface: A Molecular Dynamics Simulation Study.” **Y. Yang** and B. B. Laird. (海报展示 *Poster Presentation*)
13. The Annual Meeting of the Division of Shanghai Computational Physics Society, Shanghai, October, 2016; “Solid-Liquid Interfacial Premelting and Its Lower Dimensional Precursor.” **Y. Yang**. (邀请报告 *Invited Talk*)
14. The ECNU Physics Departmental Annual Symposium, Shanghai, December, 2016; “Solid-Liquid Interfacial Premelting and Its Lower Dimensional Precursor.” **Y. Yang**. (口头报告 *Oral Presentation*)

## 参与会议报告

1. MS&T 2008 Conference & Exhibition, Pittsburgh, Pennsylvania, United States, October, 2008; “A Theoretical and Atomistic Simulation Study of Solute Trapping.” J. J. Hoyt, **Y. Yang**, M. Asta, D. Buta and D. Y. Sun. (邀请报告 *Invited Talk*)
2. TMS 2009 Annual Meeting and Exhibition, San Francisco, California, United States, January, 2009; “A Molecular Dynamics Simulation Study of Solute Trapping During Rapid Solidification.” J. J. Hoyt, **Y. Yang**, H. Humadi, D. Buta, M. Asta and D. Y. Sun. (邀请报告 *Invited Talk*)
3. APS March Meeting 2009, Pittsburgh, Pennsylvania, United States, March, 2009; “Calculation of Excess Interfacial Entropy, Stress and Energy for Solid-Liquid Interfaces.” B. B. Laird, R. L. Davidchack, M. Asta and **Y. Yang**. (口头报告 *Oral Presentation*)
4. Sino-German Symposium on Computational Materials Science: Methods and Applications, Shanghai, China, September, 2009; “Capillary Force Induced Structural Instability in Liquid Encapsulated Elastic Circular Tubes.” D. Y. Sun, **Y. Yang**, Y. F. Gao, M. Asta and J. J. Hoyt. (邀请报告 *Invited Talk*)
5. Materials Science and Engineering 701-702 Seminars, McMaster University, Hamilton, Ontario, Canada, November, 2009; “Atomistic Study of Rapid Solidification and Solute Trapping.” H. Humadi, J. J. Hoyt, N. Provatas, M. Asta and **Y. Yang**. (口头报告 *Oral Presentation*)
6. Conference on Computational Physics, Kaoshiung, China, December, 2009; “Determination of the Solid-Liquid Interfacial Free Energy by Gibbs-Cahn Integration.” B. B. Laird, R. L. Davidchack, **Y. Yang** and M. Asta. (邀请报告 *Invited Talk*)
7. TMS 2010 Annual Meeting and Exhibition, Seattle, Washington, United States, February, 2010; “Atomistic Simulation of Segregation Coefficient of High Concentration Ni-Cu Alloys.” H. Humadi, J. J. Hoyt, M. Asta and **Y. Yang**. (海报展示 *Poster Presentation*)
8. PTM 2010 Conference on Solid-Solid Phase Transformations in Inorganic Materials, Avignon, France, June, 2010; “Molecular Dynamics Simulations of Solute Trapping and Solute Drag.” M. Asta, J. J. Hoyt, **Y. Yang**, D. Y. Sun and H. Humadi. (邀请报告 *Invited Talk*)
9. Wigner Research Centre SZFKI Seminars, Budapest, Hungary, June, 2010; “Calculating the Solid-Liquid Interfacial Free Energy by Molecular Dynamics.” B. B. Laird, R. L. Davidchack, M. Asta and **Y. Yang**. (邀请报告 *Invited Talk*)
10. 5th International Conference on Multiscale Materials Modeling, Freiburg, Germany, October, 2010; “Calculation of Solid-Liquid Interfacial Free Energies using Gibbs-Cahn Integration.” B. B. Laird, R. L. Davidchack, **Y. Yang** and M. Asta. (邀请报告 *Invited Talk*)

11. TMS 2011 Annual Meeting and Exhibition, San Diego, California, United States, February, 2011; “Molecular Dynamics Simulations of Alloy Rapid Solidification.” M. Asta, H. Humadi, **Y. Yang**, B. B. Laird, D. Y. Sun and J. J. Hoyt. (邀请报告*Invited Talk*)
12. 8th Liquid Matter Conference, Vienna, Austria, September, 2011; “Calculation of Solid-Liquid Interfacial Free Energies using Gibbs-Cahn Integration.” B. B. Laird, R. L. Davidchack, **Y. Yang** and M. Asta. (海报展示*Poster Presentation*)
13. MS&T 2011 Conference & Exhibition, Columbus, Ohio, United States, October, 2011; “Atomistic Modeling of Chemically Heterogeneous Solid-Liquid Interfaces.” M. Asta, **Y. Yang**, P. Palafox-Hernandez, D. L. Olmsted, B. B. Laird and U. Dahmen. (邀请报告*Invited Talk*)
14. APS March Meeting 2012, Boston, Massachusetts, United States, March, 2012; “Disorder Trapping During Crystallization of the B2 Ordered NiAl System.” D. Y. Sun, X. Q. Zheng, **Y. Yang**, Y. F. Gao, J. J. Hoyt and M. Asta. (口头报告*Oral Presentation*)
15. TMS 2012 Annual Meeting and Exhibition, Orlando, Florida, United States, March, 2012; “Direct Computation of the Solute Drag on a Moving Interface Using Atomistic Simulations.” J. J. Hoyt, H. Humadi, **Y. Yang**, D. Buta, B. B. Laird, D. Y. Sun and M. Asta. (邀请报告*Invited Talk*)
16. M2F2 Seminar, Department of Aerospace Engineering, University of Kansas, Lawrence, Kansas, United States, October, 2012; “Computational Materials Science and Applied Statistical Mechanics.” B. B. Laird, **Y. Yang** and M. Asta. (邀请报告*Invited Talk*)
17. Workshop on Atomistic and Mesoscale Modeling of Material Defects, Institute for Pure and Applied Mathematics (IPAM), University of California, Los Angeles, California, United States, October, 2012; “Atomistic Simulations of Chemically Heterogeneous Metal Interfaces.” B. B. Laird, P. Palafox-Hernandez, **Y. Yang** and M. Asta. (邀请报告*Invited Talk*)
18. APS March Meeting 2013, Baltimore, Maryland, United States, March, 2013; “Size dependent Melting Behavior of Iron Nanoparticles by Replica Exchange Molecular Dynamics.” Q. Shu, **Y. Yang**, Y. T. Zhai, D. Y. Sun, H. J. Xiang and X. G. Gong. (口头报告*Oral Presentation*)
19. The 8th Pacific Rim International Congress on Advanced Materials and Processing Symposium L: Modeling and Simulation of Processes, Microstructures, and Behavior, Waikoloa, Hawaii, United States, August, 2013; “Solid-Liquid Interfacial Premelting.” B. B. Laird, **Y. Yang** and M. Asta. (邀请报告*Invited Talk*)
20. TMS 2014 Annual Meeting and Exhibition, San Diego, California, United States, February, 2014; “Prefreezing and Premelting at Solid-liquid Interfaces.” B. B. Laird, P. Palafox-Hernandez, M. Asta and **Y. Yang**. (邀请报告*Invited Talk*)
21. TMS 2014 Annual Meeting and Exhibition, San Diego, California, United States, February, 2014; “Role of the Solid-liquid Interface in the Brownian Motion of Pb Inclusions in Al.” U. Dahmen, T. Radetic, E. Johnson, **Y. Yang**, D. L. Olmsted, B. B. Laird and Mark Asta. (邀请报告*Invited Talk*)
22. APS March Meeting 2014, Denver, Colorado, United States, March, 2014; “Simulation of Electric Double-Layer Capacitors: Evaluation of Constant Potential Method.” Z. X. Wang, B. B. Laird, **Y. Yang**, D. L. Olmsted and M. Asta. (口头报告*Oral Presentation*)
23. James Skinner 60th Birthday symposium, Madison, Wisconsin, United States, May, 2014; “Solid-Liquid Interfacial Premelting.” B. B. Laird, **Y. Yang** and M. Asta. (邀请报告*Invited Talk*)
24. 9th Liblice Conference on the Statistical Mechanics of Liquids, Sec Dam Lake, Czech Republic, June, 2014; “Premelting at Solid-Liquid Interfaces.” B. B. Laird, **Y. Yang** and M. Asta. (邀请报告*Invited Talk*)
25. Workshop on Structure and Dynamics of Confined Fluids, Oak Ridge National Laboratory, Tennessee, United States, July, 2014; “Solid-Liquid Interfacial Premelting.” B. B. Laird, **Y. Yang** and M. Asta. (口头报告*Oral Presentation*)

26. Workshop on Structure and Dynamics of Confined Fluids, Oak Ridge National Laboratory, Tennessee, United States, July, 2014; “Molecular Modeling of an Electric Double-Layer Capacitor.” Z. X. Wang, B. B. Laird, **Y. Yang**, D. L. Olmsted and M. Asta. (海报展示 *Poster Presentation*)
27. CMRS2015 Annual Meeting and Exhibition, Guiyang, China, July 11, 2015; “Atomistic Simulation Study on Step Free Energy of A Faceted Chemically Heterogeneous Solid-Liquid Interface.” H. T. Liang, D. Y. Sun, B. B. Laird and **Y. Yang**. (海报展示 *Poster Presentation*)
28. The Fall Chinese Physical Society Meeting, Changchun, China, September, 2015; “Atomistic Simulation Study on Step Free Energy of A Faceted Chemically Heterogeneous Solid-Liquid Interface.” H. T. Liang, D. Y. Sun, B. B. Laird and **Y. Yang**. (口头报告 *Oral Presentation*)
29. The International Chemical Congress of Pacific Basin Societies (Pacifichem) 2015, Honolulu, Hawaii, United States, December, 2015; “Spreading of Liquid Pb Droplet on an Al Surface Exhibiting Solid-Liquid Interfacial Premelting.” B. B. Laird and **Y. Yang** (邀请报告 *Invited Talk*)
30. The International Chemical Congress of Pacific Basin Societies (Pacifichem) 2015, Honolulu, Hawaii, United States, December, 2015; “Thermodynamics and Intrinsic Structure of the Al-Pb Liquid-Liquid Interface.” B. B. Laird and **Y. Yang** (邀请报告 *Invited Talk*)
31. TMS 2016 Annual Meeting and Exhibition, Nashville, Tennessee, United States, February, 2016; “Frontiers in Solidification: An MPMD Symposium in Honor of Michel Rappaz: Spreading of Liquid Pb Droplets on an Al Surface Exhibiting Solid-liquid Interfacial Premelting.” B. B. Laird and **Y. Yang**. (邀请报告 *Invited Talk*)
32. The Annual Meeting of the Division of Shanghai Computational Physics Society, Shanghai, October, 2016; “A Molecular Dynamics Study on Interfacial Liquid-Step Free Energy and Coexistence Structure at Al-Pb Solid-Liquid Interface.” H. T. Liang, D. Y. Sun, B. B. Laird and **Y. Yang**. (邀请报告 *Invited Talk*)
33. The Annual Meeting of the Division of Shanghai Computational Physics Society, Shanghai, October, 2016; “Disordering Transitions at Interfacial Liquid-Step Boundaries at A Faceted Chemically Heterogeneous Solid-Liquid Interface.” H. T. Liang and **Y. Yang**. (海报展示 *Poster Presentation*)
34. The Annual Meeting of the Division of Shanghai Computational Physics Society, Shanghai, October, 2016; “Molecular Dynamics Study of the Monolayer Confined Square Ice-Water Phase Equilibria.” H. Du and H. T. Liang and **Y. Yang**. (海报展示 *Poster Presentation*)
35. The Annual Meeting of the Division of Shanghai Computational Physics Society, Shanghai, October, 2016; “Computational Study of the Kinetic Coefficients for the Dipolar Molecular Crystal-Melt Interfaces.” X. Q. Xu and **Y. Yang**. (海报展示 *Poster Presentation*)
36. The Annual Meeting of the Division of Shanghai Computational Physics Society, Shanghai, October, 2016; “MD Study on the Surface Tension and Intrinsic Structure of Water-Vapor Surface under Electric Fields.” P. L. Yang, H. T. Liang and **Y. Yang**. (海报展示 *Poster Presentation*)
37. Materials Science and Engineering Seminars, RWTH Aachen University, Aachen, Germany, November, 2016, “Prefreezing and Premelting at Solid-Liquid Interfaces.” B. B. Laird and **Y. Yang**. (邀请报告 *Invited Talk*)