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PERSONAL DATA

Male; Born July 15, 1983 in Xinxiang, Henan, China; Married

EDUCATION

Ph.D. in Condensed Matter of Physics, East China Normal University, Shanghai, China. June, 2010

Ph.D. Exchange Program in Material Science, University of California at Davis, Davis, California, United States. January, 2008 - January, 2009

Bachelor of Science in Physics, East China Normal University, Shanghai, China. June, 2004

PROFESSIONAL EXPERIENCE

Distinguished Research Fellow September, 2014 - present
East China Normal University, Department of Physics, Shanghai, China.

Postdoctoral Associate August, 2013 - August, 2014
With Prof. Mark Asta at **University of California, Berkeley**, Department of Materials Science and Engineering, Berkeley, California, United States.

- Atomistic simulations of model electrolyte/electrode interface relevant for supercapacitor and battery applications. Research supported by the United States Department of Energy through an Energy Frontiers Research Center(EFRC). (Contract No. DE-SC0001342)

Postdoctoral Associate January, 2011 - August, 2013
With Prof. Brian B. Laird at **University of Kansas**, Department of Chemistry, Lawrence, Kansas, United States.

- Fundamental studies of chemically heterogenous and elemental solid-liquid and liquid-liquid interfaces. Research supported by the United States National Science Foundation. (Contract No. CHE0957102)

- ★ Discovered the third class of premelting transition in nature under ambient pressures. (*Phys. Rev. Lett.* 339, 452, 2013)
- ★ Devised precise atomistic simulation to uncover the role of the solid-liquid interface in the novel Brownian motion of liquid Pb inclusions in solid Al. (Collaborated with experimentalists at the United States National Center for Electron Microscopy, *manuscript in preparation*)
- ★ Revealed the spreading kinetics and multi-phase equilibrium of wetting droplet coupled with solid-liquid interfacial premelting transition. (*Manuscript in preparation*)
- ★ Atomistically resolved the intrinsic interfacial structure of Al/Pb liquid-liquid interface and validated the classical capillary wave theory for such interface. (*Invited article for special issue in J. Phys. Chem. B*, 2014)

Research Assistant

August, 2010 - January, 2011

With Prof. Xingao Gong at **Fudan University**, Department of Physics, Shanghai, China.

- Investigation into the size and structure effect on the latent heat and melting point of nanoclusters, relevant for solar energy storage devices.

Research Specialist

January, 2008 - January, 2009

With Prof. Mark Asta at **University of California, Davis**, Department of Materials Science and Engineering, Davis, California, United States.

- Atomistic simulations of rapid crystal-growth kinetics from alloy melts. Research supported by the United States Department of Energy, Office of Basic Energy Sciences. (Contract No. DE-FG02-06ER46282)
- ★ Constructed unprecedented quantitative method for atomistic modeling to analyze non-equilibrium processes on moving interfaces and to predict kinetic properties of crystal-melt interfaces. Discovered the complete solute trapping transition in rapid solidification, solved a long-time discussing problem in description of experimental data by various phenomenological models. First time calculated solute drag effects in thermodynamic driving force during crystal growth. (*Phys. Rev. Lett.* 107, 25505, 2011)

Graduate Research Assistance

July, 2004 - July, 2010

With Prof. Deyan Sun at **East China Normal University**, Department of Physics, Shanghai, China.

- Theoretical and simulation study of structure and instability of nanoscale material.
- ★ Proposed elasto-capillary theory for liquid infiltrated elastic circular tube system, revealed the geometrical nature of elasto-capillary physics in such system. Pioneered atomistic simulation as a research methodology into the field of elasto-capillarity. (*Phys. Rev. B: Rapid Communications* 81, 241407, 2010)
- ★ Constructed the theoretical model based on two universal structural parameters,

for predicting ground state structural phase diagram of nanoclusters described by simple pair potentials. (*Chem. Phys. Lett.* 474, 119, 2009)

PROFESSIONAL SOCIETY MEMBERSHIPS

American Physical Society (APS)

The Royal Society of Chemistry (RSC)

HONOR SOCIETIES, AWARDS and FELLOWSHIPS

Excellent Doctoral Dissertation Award of Shanghai City: Awarded as one of nine excellent doctoral dissertations in physics, 2012

Funded by the Institute for Pure and Applied Mathematics (IPAM) at University of California, Los Angeles: For attending the workshop on atomistic and mesoscale modeling of materials defects, 2012

Selected to attend Energy Frontier Research Centers (EFRC) summer school at Oak Ridge National Laboratory on defects, deformation and damage in structural materials, 2012

China Scholarship Council Scholarship: For conducting academic cooperation under joint-PhD-training programs at world-class university, 2008

TEACHING EXPERIENCE

East China Normal University

- Fall 2016: Graduate Course: Advanced Solid State Physics.
- Fall 2016: Mentor, ECNU Undergraduate Elite Program.

NATIONAL AND INTERNATIONAL SERVICE

Referee of manuscripts for Computational Material Science

Referee of manuscripts for Rare Metals

RESEARCH KEYWORDS

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.

RESEARCH INTERESTS

Yang Yang's research interests focus on: i) Structure, statistical thermodynamics and kinetic theory of bulk model materials (vapor, liquid and solid) (pure and binary mixture substances) and their interfaces. Studies are carried out by coupling atomistic simulations with theoretical models, and by employing the state of the art characterization for the interfacial structures. ii) Thermodynamics, structural phase diagram of nanomaterials; diffusion and wetting/spreading kinetics of nanodroplets; elasto-capillarity at nanometer-scale limit. Studies are carried out by coupling atomistic simulations with theoretical models. iii) Fundamental investigations into electrode(charged metal)-liquid interfaces. To incorporate molecular level understanding of electrochemical, electrokinetic and electrolytic behavior into the traditional understanding of this type of interface, and to derive insights into the factors that contribute to high performance in high energy density batteries and supercapacitors.

CURRENT FUNDING

Zhejiang Youth Scholars Programme Startup Funding, ¥1,000,000, September, 2014 - July, 2019, Yang Yang, PI

National Natural Science Foundation of China (Grant No. 11504110), ¥200,000, January, 2016 - December, 2018, Yang Yang, PI

PUBLICATIONS (20 Listed)

I. Thermodynamics and Kinetics of the Interfaces

1. 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).
2. 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). *Selected as one of ten manuscripts included in list of Modelling and Simulation in Materials Science and Engineering "Highlights of 2010."*
3. 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).
4. 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).
5. **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, 4, (2011). *Included as Chapter 17 in the Book "Solidification of Containerless Undercooled Melts" . Editors: D. M. Herlach and D. M. Matson, 2012, Wiley-VCH Verlag & Co. KGaA, Boschstr. 12, 69469, Weinheim, Germany*
6. 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).
 7. **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).
 8. 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).
 9. **Y. Yang**, M. Asta and B. B. Laird, "Solid-Liquid Interfacial Premelting", *Phys. Rev. Lett.*, 110, 096102, (2013).
 10. **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). *Invited Article in The Journal of Physical Chemistry*
 11. H. Y. Zhang, F. Liu, **Y. Yang** and D. Y. Sun, "Molecular Dynamics Study of Defect Trapping during Crystallization of Small Undercooled FCC Ni and FCC Al", *To be submitted to Phys. Rev. B*, (2015).
 12. X. Q. Zheng, **Y. Yang**, J. J. Hoyt, M. Asta and D. Y. Sun, "Atomistic Characterization of the B2 Ordered NiAl Solid-Liquid Interface", *To be submitted to Scripta Materialia*, (2015).

II. Thermodynamics, Structure and Elasto-Capillarity of Nanomaterials, Diffusion and Spreading Kinetics of Nanodroplets

1. **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).
2. **Y. Yang** and D. Y. Sun, "Effect of the Equilibrium Pair Separation on Cluster Structures", *Commun. Comput. Phys.*, 6, 730, (2009).
3. **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*, 81, 241407, (2010). *Rapid Communications*.
4. 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).
5. 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).
6. 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).

7. T. Radetic, E. Johnson, D. L. Olmsted, **Y. Yang**, B. B. Laird, M. Asta and U. Dahmen, "Step-Controlled Brownian Motion of Nanosized Liquid Pb Inclusions in a Solid Al Matrix", Submitted to Nature Material, (2014).

III. Electrokinetics and Electrochemistry at Electrode-Electrolyte Interfaces

1. Z. X. Wang, B. B. Laird, **Y. Yang**, D. L. Olmsted and M. Asta, "Evaluation of Constant Potential Method in Simulating Electric Double-Layer Capacitors", J. Chem. Phys., 141, 184102, (2014). *Chosen as the journal cover featured article in Volume 141 Issue 18 on November 14. Selected in the 2014 JCP Editors Choice Collection.*

(INVITED) LECTURES/PRESENTATIONS

1. The Fall Chinese Physical Society Meeting, Beijing, China, September, 2006; "The Classification of Cluster Structure." **Y. Yang** and D. Y. Sun. (*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. (*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. J. Hoyt, B. B. Laird and M. Asta. (*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. (*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. (*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. (*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. (*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. (*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. (*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. (*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. (*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. (*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 (*Invited Talk*)
14. The ECNU Physics Departmental Annual Symposium, Shanghai, December, 2016; “Solid-Liquid Interfacial Premelting and Its Lower Dimensional Precursor” Y. Yang (*Oral Presentation*)

CONTRIBUTED LECTURES/PRESENTATIONS

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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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**. (*Contributed 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. (*Contributed 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**. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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**. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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. (*Contributed 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**. (*Contributed Poster Presentation*)
 28. The Fall Chinese Physical Society Meeting, Changchun, China, September, 2015; “Atomistic Simulation Study on Step Free Energy of A Faceted Chemically Hetero-

- geneous Solid-Liquid Interface.” H. T. Liang, D. Y. Sun, B. B. Laird and **Y. Yang**. (*Contributed 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**. (*Contributed 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**. (*Contributed 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**. (*Contributed 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 and **Y. Yang**. (*Contributed 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**. (*Contributed 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, H. T. Liang and **Y. Yang**. (*Contributed 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**. (*Contributed 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**. (*Contributed 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**. (*Contributed Invited Talk*)