



Liyi Bai(白丽宜)

Pusan National University, Computational Materials

"AI + Materials"

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Education and Academic Positions

Westlake University

2021.04-Present

Postdoctoral Fellow, Department of Physics, Mentor: Prof. Shi Liu

China · Hangzhou

Pusan National University

2015.09-2021.02

Ph.D. Nanofusion Technology, Adviser: Joonkyung Jang

South Korea · Busan

- Thesis: "Theoretical and Computational Investigation on Hydration Layer Probed by Atomic Force Microscopy."

Zhongyuan University of Technology

2011.09-2015.07

B.S. Polymer Materials and Engineering, Graduated with Honors, GPA: 86/100

China · Zhengzhou

Research experience

- AI4Science, Classical Molecular Dynamics, ab initio MD, DPMD, DFT
- Machine learning potential development and ion transport characterization of ternary high-pressure water-based lithium-ion electrolytes
- Machine learning potential development and polarization reversal dynamics in two-dimensional ferroelectric materials
- Molecular simulation on the phase, structure and dynamics of hydration layer
- Theory and simulation of spectroscopies of liquid/solid, liquid/air interfacial structure (sum frequency generation spectroscopy, Raman, IR)
- Phase behavior in confined system (design of super-hydrophobic surfaces)

Work experience

"Computer Simulation with LAMMPS", PNU Summer School

2018.08 / 2017.07

Lecturer

Korea · Busan

Institute of High Energy Physics Chinese Academy of Sciences

2016.06-2016.07

Visiting student, Prof. Gao Xinfu's Group

China · Beijing

Project experience

1. Design and Development of Air-Stable High-Voltage Lithium Batteries, Funded by Future Industry Research Project of West Lake University (2022.12-2024.12, 200 RMB)
2. Theoretical Study of Two-Dimensional Ferroelectric Polarization Reversal Characteristics, National Natural Science Foundation" (2021.1-2023.12, 24 RMB)

3. Study on the Contact Mechanics of an Atomic Force Microscope Tip, National Research Foundation of Republic of Korea. (2016.5-2018.4)
4. Phase Transitions in Confined Systems, National Research Foundation of Republic of Korea. (2015.5-2019.4)

Awards

- Postgraduate scholarship, Pusan National University, Sep. 2015 - Feb. 2019
- BK21 scholarship, Ministry of Education, Republic of Korea, Sep. 2016
- Fully funded Ph.D. scholarship, National Research Foundation of Republic of Korea, Sep. 2015 - Feb. 2021
- National encouragement scholarship, Ministry of Education, P. R. China, Nov. 2014
- National encouragement scholarship, Ministry of Education, P. R. China, Nov. 2013
- Merit Students, Zhongyuan University of Technology, Dec. 2013

Presentations

1. Poster presentation “Phase, Structure, and Dynamics of the Hydration Layer Probed by Atomic Force Microscopy”, KCS-PyhsChem Summer Symposium. (2019.7.8-10)
2. Oral presentation “Dewetting Transition of Water Confined between Atomically Rough Surfaces”, Japan-Korea Student Workshop: Hiroshima University and Pusan National University. (2018.11.15-17, Hiroshima University, Japan)
3. Poster presentation “Dewetting Transition of Water Confined between Atomically Rough Surfaces”, KCSPyhsChem Summer Symposium. (2018-7.9-11)
4. Poster presentation “Structure and Dynamics Study of Interface Water Molecules under Confinement”, The 12th National Conference on Soft Matter and Biophysical Physics (2022.10.29-30, Zhejiang · Wenzhou)

Publications

Google Scholar: <https://scholar.google.co.uk/citations?user=T4TaoM0AAAAJ&hl=en&oi=ao>

1. **Bai, L. et al.** Deep Learning of Accurate Force Field of High Voltage Water-in-salt Electrolytes. *In Preparation.*
2. **Bai, L. et al.** Ab initio Molecular Dynamics Study on Vibrational Sum Frequency Generation of Water at Hydrophobic/hydrophilic Surfaces. *In Preparation.*
3. **Bai, L.** C. Ke, T. Zhu, S. Liu.(2023). Intrinsic ferroelectric switching in two dimensions. **arXiv**. DOI:10.48550/arXiv.2307.09211.
4. Wu, J., **Bai, L.(co-first author)**, Huang, J., Ma, L., Liu, J., Liu, S. (2021). Accurate Force Field of Two dimensional Ferroelectrics from Deep Learning. *Physical Review B*, 104(17), 174107. (JCR: Q1)
5. **Bai, L.**, Kim, K., Ha, M. Y., Ahn, Y., Jang, J. (2021). Molecular Insights on the Wetting Behavior of a Surface Corrugated with Nanoscale Domed Pillars. *Langmuir* 37, 31, 9336–9345. (JCR: Q1)

6. Zhang, Z., **Bai, L.(co-first author)**, Chung, S., Jang, J. (2021). Effects of the Wettability of a Probing Tip on the Hydration Layer Imaged in Atomic Force Microscopy. *The Journal of Physical Chemistry C*, 125, 11197–11205. (JCR: Q1)
7. **Bai, L.**, Zhang, Z., Jang, J. (2019). Phase, Structure, and Dynamics of the Hydration Layer Probed by Atomic Force Microscopy. *The Journal of Physical Chemistry C*, 123(35), 21528-21537. (JCR: Q1)
8. **Bai, L.**, Jang, J., Zhang, Z., Jang, J. (2018). Dewetting transition of water confined between atomically rough surfaces: A lattice gas Monte Carlo simulation study. *Chemical Physics Letters*, 694, 29-34. (JCR: Q2)
9. Zhao, M., **Bai, L.**, Jang, J. (2020). Underwater adhesion of mussel foot protein on a graphite surface. *Applied Surface Science*, 511, 145589. (JCR: Q1)
10. Kim, K., Choi, S., Zhang, Z., **Bai, L.**, Chung, S., Jang, J. (2022). Molecular Features of Hydration Layers: Insights from Simulation, Microscopy, and Spectroscopy. *The Journal of Physical Chemistry C*.126(21), 8967–8977. (JCR: Q1)

Skills

Programming Languages/Tools	Fortran, Matlab, Python, Bash, \LaTeX , Markdown
Simulation Software/Tools	LAMMPS, VMD, VASP, CP2K, Materials Studio, Packmol, VESTA, OVITO, DPGEN
Deep Learning	DeepMD-Kit, Keras