Liyi Bai(白丽宜)

Computational Materials, Pusan National University
"AI + Materials"
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Education and Academic Positions

Westlake University *2021.04-Present*
Postdoctoral Fellow, Department of Physics, Mentor: Prof. Shi Liu *Hangzhou · China*

Pusan National University *2015.09-2021.02*
Ph.D. Nanofusion Technology, Adviser:Joonkyung Jang *Busan · Korea*

- *Thesis: "Theoretical and Computational Investigation on Hydration Layer Probed by AtomicForce Microscopy."*

Zhongyuan University of Technology *2011.09-2015.07*
B.S. Polymer Materials and Engineering, Graduated with Honors, GPA:86/100 *Zhengzhou · China*

Research Experience

- **AI4Science, Classical Molecular Dynamics, ab initial MD, DPMD, DFT**
- Machine learning potential development and ion transport characterization of ternary high-pressure water-based lithium-ion wlectrolytes
- 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 *Busan · Korea*

Institute of High Energy Physics Chinese Academy of Sciences *2016.06-2016.07*
Visiting student, Prof. Gao Xinfa's Group *Beijing · China*

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*, RMB: 2 000 000)

2. Theoretical Study of Two-Dimensional Ferroelectric Polarization Reversal Characteristics, National Natural Science Foundation" (*2021.1-2023.12*, RMB: 240 000)

3. Study on the Contact Mechanics of an Atomic Force Microscope Tip, National Research Foundation of Republic of Korea. (*2016.05-2018.04*)

4. Phase Transitions in Confined Systems, National Research Foundation of Republic of Korea. (*2015.05-2019.04*)

Awards

- Fully funded Ph.D. scholarship, National Research Foundation of Republic of Korea, *2015.09 - 2021.02*
- Postgraduate scholarship, Pusan National University, *2015.09 - 2019.02*
- BK21 scholarship, Ministry of Education,Republic of Korea, *2016.09*
- National encouragement scholarship, Ministry of Education, P. R. China, *2014.11*
- National encouragement scholarship, Ministry of Education, P. R. China, *2013.11*
- Merit Students, Zhongyuan University of Technology, *2013.12*

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*, Busan · Korea)

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*, Busan · Korea)

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*, Wenzhou · Zhejiang)

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