Zhu, Jia-Xin

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https://github.com/ChiahsinChu

EDUCATION

2020 – present **Ph.D. candidate in Chemistry**

College of Chemistry and Chemical Engineering, Xiamen University

2016 – 2020 **B.Sc. in Chemistry**

College of Chemistry and Chemical Engineering, Xiamen University

- GPA 3.85/4.0 (top 5%)
- Excellent Graduates in Xiamen University (2020)
- National Scholarship (2017)

RESEARCH INTEREST

Electrified solid/liquid interfaces are the key to many physicochemical processes in a myriad of areas including electrochemistry and colloid science. For a molecular-level understanding of electric double layers, ab initial molecular dynamics (AIMD) simulation can be utilised. Despite the great successes achieved by AIMD, this method suffers from the limited timescale and cell size due to high computational cost. What's more, the determination of pH, another essential quantity of the electrochemical system, is unaffordable. In my Ph.D. project, I aim to **simulate the electrochemical interfaces under certain conditions (i.e., pH and electrode potential) based on machine learnt potential (MLP)**.

RESEARCH EXPERIENCES

Oct. 2022 – Apr. 2023 **Ph.D. visiting project at Leiden University (LU)**

I performed research on the dielectric properties on Pt/water interfaces, under the supervision of Prof. Marc Koper (LU), Dr. Katharina Doblhoff-Dier (LU) and Prof. Jun Cheng (XMU). Particularly, machine-learnt potentials (MLP) will be utilised to achieve a timescale up to the nanosecond when keeping the ab initio accuracy.

Oct. 2019 – Mar. 2020 **Final year project of B.Sc. at Leiden University (LU)**

I performed research on the interfacial structures and potential of the (electrified) Pt(100)/water interface, under the supervision of Prof. Marc Koper (LU), Dr. Katharina Doblhoff-Dier (LU), Prof. Jun Cheng (XMU) and Dr. Jia-Bo Le (XMU). This work has been published in *Journal of Physical Chemistry C* (DOI: 10.1021/acs.jpcc.1c04895).

Jul. 2019 **Summer School France Excellence 2019 (France - China)**

Sustainable Catalysis: from Fundamental Science to Industrial Practice (University of Lille)

Dec. 2018 – Dec. 2019 **Undergraduate training program at Xiamen University (XMU)**

I performed research on the level alignment of CdTe(100)/water interface, under the supervision of Prof. Jun Cheng. In this project, I learnt how to perform the DFT calculation in CP2K, and analyse the data with Python.

PUBLICATIONS

- **Zhu, J.-X.**, Le, J.-B., Koper, M. T. M., Doblhoff-Dier, K.*, and Cheng, J.* Effects of Adsorbed OH on Pt(100)/Water Interfacial Structures and Potential. *Journal of Physical Chemistry C*, **2021**, *125*, 21571. https://doi.org/10.1021/acs.jpcc.1c04895
- Li, X.-Y., Chen, A., Yang, X.-H., **Zhu, J.-X.**, Le, J.-B.*, and Cheng, J.* Linear Correlation between Water Adsorption Energies and Volta Potential Differences for Metal/water Interfaces. *Journal of Physical Chemistry Letters*, **2021**, *12*, 7299. https://doi.org/10.1021/acs.jpclett.1c02001
- Yang, X.-H., Zhuang, Y.-B., **Zhu, J.-X.**, Le, J.-B., and Cheng, J.* Recent progress on multiscale modeling of electrochemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2022**, *12*, e1559. https://doi.org/10.1002/wcms.1559
- Zhou, W., Li, L., Qin, R., **Zhu, J.-X.**, Liu, S., Mo, S., Shi, Z., Fang, H., Ruan, P., Cheng, J., Fu, G.*, and Zheng, N.* Non-Contact Biomimetic Mechanism for Selective Hydrogenation of Nitroaromatics on Heterogeneous Metal Nanocatalysts. *Science China Chemistry*, **2022**, *65*, 726. https://doi.org/10.1007/s11426-021-1198-2
- Zeng, J.; Zhang, D.; Lu, D.; Mo, P.; Li, Z.; Chen, Y.; Rynik, M.; Huang, L.; Li, Z.; Shi, S.; Wang, Y.; Ye, H.; Tuo, P.; Yang, J.; Ding, Y.; Li, Y.; Tisi, D.; Zeng, Q.; Bao, H.; Xia, Y.; Huang, J.; Muraoka, K.; Wang, Y.; Chang, J.; Yuan, F.; Bore, S. L.; Cai, C.; Lin, Y.; Wang, B.; Xu, J.; **Zhu, J.-X.**; Luo, C.; Zhang, Y.; Goodall, R. E. A.; Liang, W.; Singh, A. K.; Yao, S.; Zhang, J.; Wentzcovitch, R.; Han, J.; Liu, J.; Jia, W.; York, D. M.; E, W.; Car, R.; Zhang, L.; Wang, H. DeePMD-Kit v2: A Software Package for Deep Potential Models. *The Journal of Chemical Physics* **2023**, *159*, 054801. https://doi.org/10.1063/5.0155600.

ACADEMIC CONFERENCES

- The 74th Annual Meeting of the International Society of Electrochemistry (ISE), **poster presentation** (Lyon, France, Sep. 2023)
- The 73rd Annual Meeting of the International Society of Electrochemistry (ISE), **oral presentation** (online, Sep. 2022)
- The 72nd Annual Meeting of the International Society of Electrochemistry (ISE), **oral presentation** (online, Aug. 2021)
- NSFC-BC Researcher Links Workshop on "Electrochemistry for Energy Applications: Experiment Meets Theory" (online, May 2021)
- The 32nd Chinese Chemical Society (CCS) congress, **poster presentation** (Zhuhai, China, Apr. 2021)
- 708. WE-Heraeus-Seminar on "Operando surface science – Atomistic insights into electrified solid/liquid interfaces", **poster presentation** (Physikzentrum Bad Honnef, Germany, Dec. 2019)
- Computational Chemistry Workshop (Xiamen, China, Sep. 2019)

SKILLS

Languages: Chinese – Fluent
English – Intermediate
- *IELTS* 7.5 (Reading 9.0 Listening 8.0 Writing 6.5 Speaking 6.0)

Programming Languages: Python, Fortran, C++

Software: CP2K, VASP, Lammps, DeepMD-kit