Jiapeng Liu

Contact Information

Rm 4225B, 4/F (Lift 24)
Department of Mechanical and Aerospace Engineering
Hong Kong University of Science and Technology
Clear Water Bay, Hong Kong

Tel: (+852) 51687140
(+86) 17324487051
E-mail: jliubt@connect.ust.hk
Web: jiapeng-liu.github.io

Education

Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong

Ph.D., Mechanical Engineering — Sep, 2016-Aug, 2020

- Dissertation: "Computational and experimental perspectives for the development of solid state ionics for energy storage systems"
- Supervisor: Francesco Ciucci, Fellow of the Royal Society of Chemistry

Northwestern Polytechnical University, Xi'an, China

B.Eng., Thermal Energy and Power Engineering — Sep, 2009-Jul, 2013

Research Interests

Investigating the transport phenomenon in energy materials via

- Molecular Dynamics (MD)
- Density Functional Theory (DFT)
- Finite Element Method (FEM)

Developing next-generation clean energy conversion systems, including

- Solid Oxide Fuel Cell (SOFC)
- Protonic Ceramic Fuel Cell (PCFC)
- Solid-State Lithium-ion Battery (SSLIB)

Applying deep learning frameworks in areas as

- Physics-informed Neural Network for State of Healthy (SOH) of LIB
- Graph Neural Network for Crystal Properties
- Distribution of Relaxation Times for Electrochemical Impedance Spectroscopy

Honors and Awards

Travel Grant Recipient of Solid State Ionic-22	2019
Post Graduate Scholarship of Hong Kong University of Science and Technology	2016-2020
Outstanding Graduate of Northwestern Polytechnical University	2013
National Encouragement Scholarship & Merit Award	2010-2013
First Prize of Advanced Mathematics Contest for Undergraduate in Shaanxi	2010, 2012
First Prize of National Mathematical Modeling Contest in Shaanxi	2011
Third Prize of International Mathematical Contest In Modeling	2012

Academic Experience

Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong

Postdoctoral Fellow — Oct, 2020 - Sep, 2021

Project: Development of a Meta-solid-state Electrolyte in Li-ion Batteries

- Design and develop solid-state lithium-ion batteries with a special focus on reducing the contact resistance between the electrode|electrolyte interface.
- Construct deep learning models to predict the state of health for lithium-ion batteries.
- Propose graph neural networks to predict the properties of crystals and assist the high-throughput search for desired functional materials.

Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong

Ph.D. Candidate — Sep, 2016 - Aug, 2020

- First-principles predictions of Li^+ transportation mechanisms, electrochemical window, the thermodynamic stability of solid electrolytes.
- Development of new and high-performance perovskite-type cathode materials for solid oxide fuel cells by combining both experiments and theoretical calculations.
- Deconvolving the electrochemical impedance spectroscopy to obtain the distribution of relaxation times via Gaussian Process, deep Neural Network, and other statistical approaches.
- Modeling the transport behaviors of polarons, oxygen vacancies in mixed ionic-electronic conductors by solving the Poisson-Nernst–Planck equation with finite element method.

City University of Hong Kong, 83 Tat Chee Ave, Kowloon Tong, Hong Kong

Research Assistant Mar, 2015 - Jul, 2016

Project: Continuous Monitoring of Roadside Air Quality in Hong Kong

- Developed a neural network model to predict the roadside air quality in the North District of Hong Kong (N.D.), including the concentration change trends of NO, NO_2, O_3, etc.
- Designed experiments to improve the monitoring performance of chemical sensors and accurately capture changes in air quality.

Xi'an Jiaotong University, No. 28, Xianning West Road, Xi'an, China

Research Assistant Jun, 2013 - Nov, 2014

Project: Numerical Simulation of Supercritical CO_2 Heat Pump System

- Independently carried out numerical simulations for heat transfer problems in supercritical CO_2 heat pump systems, and developed a new numerical algorithm to simulate and predict the cooling process in gas coolers.
- Independently designed and developed the C++ based software for simulating and analyzing CO_2 heat pump systems and finalized the report.

Publications

†: co-first author; ⋆: corresponding author

1. **Liu, J.**, Lu, Z., Effat, M. B., and Ciucci, F.⋆, 2019. A theoretical study on the stability and ionic conductivity of the $Na_{11}M_2PS_{12}$ (M= Sn, Ge) superionic conductors. ***Journal of Power Sources***, 409, 94-101. DOI: 10.1016/j.jpowsour.2018.10.077 (IF=9.127)
2. **Liu, J.**, and Ciucci, F.⋆, 2017. Modeling the impedance spectra of mixed conducting thin films with exposed and embedded current collectors. ***Physical Chemistry Chemical Physics***, 19(38), 26310-26321. DOI: 10.1039/C7CP03703A (IF=3.676)
3. **Liu, J.**, Wang, J., Belotti, A. and Ciucci, F.⋆, 2019. P-substituted $Ba_{0.95}La_{0.05}FeO_{3-\delta}$ as a cathode material for SOFCs. ***ACS Applied Energy Materials***, 2(8), 5472-5480. DOI: 10.1021/acsaem.9b00624 (IF=6.024)
4. **Liu, J.**, and Ciucci, F.⋆, 2019. The Gaussian process distribution of relaxation times: A machine learning tool for the analysis and prediction of electrochemical impedance spectroscopy data. ***Electrochimica Acta***, 331, 135316. DOI: 10.1016/j.electacta.2019.135316 (IF=6.901)
5. **Liu, J.**, and Ciucci, F.⋆, 2020. The deep-prior distribution of relaxation times. ***Journal of The Electrochemical Society***, 167, 026506. DOI: 10.1149/1945-7111/ab631a (IF=4.316)
6. **Liu, J.**†, Wan, T. H.†, and Ciucci, F.⋆, 2020. A Bayesian view on the Hilbert transform and the Kramers-Kronig transform of electrochemical impedance data: probabilistic estimates and quality scores. ***Electrochimica Acta***, 357, 136864. DOI: 10.1016/j.electacta.2020.136864 (IF=6.901)
7. Zhang, Z.†, **Liu, J.**†, Wang, J.†, Wang, Q., Wang, Y., Wang, K., Wang, Z., Gu, M., Tang, Z., Lim, J., Zhao, T., and Ciucci, F.⋆. Single-atom catalyst for high-performance methanol oxidation. ***Nature Communications***, *Accepted.* (co-first author)
8. Lin, X.†, Zhou, G.†, **Liu, J.**†, Yu, J., Effat, M. B., Wu, J., and Ciucci, F.⋆, 2020. Rechargeable battery electrolytes capable of operating over wide temperature windows and delivering high

safety. ***Advanced Energy Materials***, 2001235. DOI: 10.1002/aenm.202001235 (co-first author) (IF=29.368)

9. Song, Y.†, **Liu, J.**†, Wang, Y.⋆, Guan, D., Zhang, Z., Shao, Z.⋆, Ciucci, F.⋆. Nanocomposites: A New Opportunity for Developing Highly Active and Durable Bifunctional Air Electrodes for-Reversible Protonic Ceramic Cells. ***Advanced Energy Materials***, *Accepted*. (co-first author)
10. Lin, X.†, Zhou, G.†, **Liu, J.**†, Robson, M. J., Yu, J., Wang, Y., Zhang, Z., Kwok, S. C., and Ciucci F.⋆, 2021. Bifunctional hydrated gel electrolyte for long-cycling Zn-ion battery with NASICON-type cathode. ***Advanced Functional Materials***, *Accepted*. (co-first author)
11. Zhang, Z.†, **Liu, J.**†, Curcio, A., Wang, Y., Wu, J., Zhou, G., Tang, Z., and Ciucci, F.⋆, 2020. Atomically dispersed materials for rechargeable batteries. ***Nano Energy***, 76, 105085. DOI: 10.1016/j.nanoen.2020.105085 (co-first author) (IF=17.881)
12. Kim, J. H.†, Kim, J. K.†, **Liu, J.**†, Curcio, A., Jang, J. S., Kim, I. D., Ciucci, F.⋆, and Jung, W.⋆, 2020. Nanoparticle ex-solution for supported catalysts: Materials design, mechanism and future perspectives. ***ACS Nano***, DOI: 10.1021/acsnano.0c07105. (co-first author) (IF=15.881)
13. Wang, K.†, **Liu, J.**†, Tang, Z.⋆, Li, L., Wang, Z., Ciucci, F.⋆, Thomsen, L. Wright, J., Chen, S., and Bedford, N.⋆, 2021. Establishing structure/property relationships in atomically dispersed Co-Fe dual site M-Nx catalysts on mesoporous carbon for oxygen reduction reaction. ***Journal of Materials Chemistry A***, 2021. DOI: 10.1039/D1TA02925H (co-first author) (HOT Paper) (IF=12.732)
14. Wang, J.⋆, Kim S. J., **Liu, J.**, Gao, Y., Choi, S., Han, J., Shin, H., Jo, S., Kim, J., Ciucci, F., Kim, H., Li, Q., Yang, W., Long, X., Yang, S.⋆, Cho, S. P., Chae, K. H., Kim, M. G., Kim, H.⋆, and Lim, J.⋆, 2021. Redirecting dynamic surface restructuring of a layered transition metal oxide catalyst for superior water oxidation. ***Nature Catalysis***, 1-11. DOI: 10.1038/s41929-021-00578-1
15. Lu, Z., **Liu, J.**, and Ciucci, F.⋆, 2020. Superionic conduction in low-dimensional-networked anti-perovskites. ***Energy Storage Materials***, 28, 146-152. DOI: 10.1016/j.ensm.2020.03.005
16. Wang, H., **Liu, J.**, Li, Q., Zhang, J., Xing, H., Wei, P., Sun, J., Ciucci, F., Lam, J.W., Lu, R.⋆, and Tang, B.Z.⋆, 2020. Positive/negative phototropism: Controllable molecular actuators with different bending behavior. ***CCS Chemistry***, 1491-1500. DOI: 10.31635/ccschem.020.202000350
17. Wang, J., Gao, Y., Chen, D., **Liu, J.**, Zhang, Z., Shao, Z., and Ciucci, F.⋆, 2017. Water splitting with an enhanced bifunctional double perovskite. ***ACS Catalysis***, 8(1), 364-371. DOI: 10.1021/acscatal.7b02650
18. Sadighi, Z., **Liu, J.**, Zhao, L., Ciucci, F., and Kim, J. K.⋆, 2018. Metallic MoS_2 nanosheets: multifunctional electrocatalyst for the ORR, OER and Li–O_2 batteries. ***Nanoscale***, 10(47), 22549-22559. DOI: 10.1039/C8NR07106C
19. Sadighi, Z., **Liu, J.**, Ciucci, F., and Kim, J. K.⋆, 2018. Mesoporous $MnCo_2S_4$ nanosheet arrays as an efficient catalyst for Li–O_2 batteries. ***Nanoscale***, 10(33), 15588-15599. DOI: 10.1039/C8NR03942A
20. Wu, J., **Liu, J.**, Lu, Z., Lin, K., Lyu, Y. Q., Li, B., Ciucci, F.⋆, and Kim, J.K.⋆, 2019. Nonflammable electrolyte for dendrite-free sodium-sulfur battery. ***Energy Storage Materials***, 23, 8-16. DOI: 10.1016/j.ensm.2019.05.045
21. Yu, J., Lyu, Y. Q., **Liu, J.**, Effat, M. B., Kwok, S. C., Wu, J., and Ciucci, F.⋆, 2019. Enabling nonflammable Li-metal batteries via electrolyte functionalization and interface engineering. ***Journal of Materials Chemistry A***, 7(30), 17995-18002. DOI: 10.1039/C9TA03784E
22. Wu, J., **Liu, J.**, Cui, J., Yao, S., Haq, M. I. U., Mubarak, N., Quattrocchi, E., Ciucci, F.⋆, and Kim, J.K.⋆, 2020. Dual-phase MoS_2 as a high-performance sodium-ion battery anode. ***Journal of Materials Chemistry A***, 8, 2114-2122. DOI: 10.1039/C9TA11913B

23. Wu, J., Yu, J., **Liu, J.**, Cui, J., Yao, S., Haq, M. I. U., Mubarak, N., Susca, A., Ciucci, F.*, and Kim, J.K.*, 2020. $MoSe_2$ nanosheets embedded in nitrogen/phosphorus co-doped carbon/graphene composite anodes for ultrafast sodium storage. ***Journal of Power Sources***, 476, 228660. DOI: 10.1016/j.jpowsour.2020.228660

24. Dai, Z., Yu, J., **Liu, J.**, Liu, R., Sun, Q., Chen, D.*, and Ciucci, F.*, 2020. Highly conductive and nonflammable composite polymer electrolytes for rechargeable quasi-solid-state Li-metal batteries. ***Journal of Power Sources***, 464, 228182. DOI: 10.1016/j.jpowsour.2020.228182

25. Susca, A., **Liu, J.**, Cui, J., Mubarak, N., Wu, J., Haq, M. I. U., Ciucci, F., and Kim, J.K.*, 2020. Affinity-engineered carbon nanofibers as scaffold for Na metal anodes. ***Journal of Materials Chemistry A***, 8, 14757-14768. DOI: 10.1039/D0TA05298A

26. Zhou, G., Lin, X., **Liu, J.**, Yu, J., Wu, J., Law, H. M., Wang, Z., and Ciucci, F.*, 2020. In situ formation of poly (butyl acrylate)-based non-flammable elastic quasi-solid electrolyte for dendrite-free flexible lithium metal batteries with long cycle life for wearable devices. ***Energy Storage Materials***, 34, 629-639. DOI: 10.1016/j.ensm.2020.10.012

27. Effat, M. B., **Liu, J.**, Lu, Z., Wan, T. H., Curcio, A., and Ciucci, F.*, 2020. The stability, elastic properties, and the Li transport mechanism of the protonated and fluorinated anti-perovskite lithium conductors. ***ACS Applied Materials & Interfaces***, 12(49), 55011–55022. DOI: 10.1021/acsami.0c17975

28. Yu, J., **Liu, J.**, Lin, X., Law, H. M., Zhou, G., Kwok, S. C., Robson, M. J., Wu, J., and Ciucci, F.*, 2021. A solid-like dual-salt polymer electrolyte for Li-metal batteries capable of stable operation over an extended temperature range. ***Energy Storage Materials***, 37, 609-618. DOI: 10.1016/j.ensm.2021.02.045

29. Belotti, A., **Liu, J.**, Curcio, A., Wang, J., Wang, Z., Quattrocchi, E., Effat, M. B., and Ciucci, F.*, 2021. Introducing Ag in $Ba_{0.9}La_{0.1}FeO_{3-\delta}$: combining cationic substitution with metal particles decoration. ***Materials Reports: Energy***, 100018. DOI: 10.1016/j.matre.2021.100018

Teaching Experience

Hong Kong University of Science and Technology

Teaching Assistant in Mechanical Engineering — Spring 2018

- MECH 2520 Design and Manufacturing, Instructor: Michael Yu WANG

Skills

- Experiment: Solid-State Battery, Solid Oxide Fuel Cell
- Professional: VASP, CP2K, Gaussian, LAMMPS, GROMACS, Pytorch, Tensorflow
- Programming: Python, Matlab, C++, Unix shell scripts
- Applications: Linux, LaTeX
- Language: English, Japanese

Referees

Francesco Ciucci (Ph.D. Advisor)
Associate Professor
Dept. MAE, HKUST
E-mail: mefrank@ust.hk

Ben Zhong Tang
Stephen K. C. Cheong Professor
Dept. Chem., HKUST
E-mail: tangbenz@ust.hk