

# Jiapeng Liu

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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	<i>Tel:</i> (+852) 5168-7140 (+86) 173-244-87051 <i>E-mail:</i> jliubt@connect.ust.hk <i>Web:</i> jiapeng-liu.github.io
EDUCATION	<b>Hong Kong University of Science and Technology</b> , Clear Water Bay, Hong Kong Ph.D., Mechanical Engineering Aug. 2020 <ul style="list-style-type: none"><li>• Dissertation: “Computational and experimental perspectives for the development of solid state ionics for energy storage systems”</li><li>• Supervisor: Francesco Ciucci, Fellow of the Royal Society of Chemistry</li></ul> <b>Northwestern Polytechnical University</b> , Xi’an, China B.Eng., Thermal Energy and Power Engineering Jul. 2013	
RESEARCH INTERESTS	Investigating the transport phenomenon in energy materials via <ul style="list-style-type: none"><li>• Density Functional Theory (DFT)</li><li>• Molecular Dynamics (MD)</li><li>• Finite Element Method (FEM)</li></ul> Developing next-generation clean energy conversion systems, including <ul style="list-style-type: none"><li>• Solid-State Lithium-ion Battery (SSLIB)</li><li>• Solid Oxide Fuel Cell (SOFC)</li><li>• Protonic Ceramic Fuel Cell (PCFC)</li></ul> Applying deep learning frameworks in areas as <ul style="list-style-type: none"><li>• Physics-informed Neural Network for State of Healthy (SOH) of LIB</li><li>• Graph Neural Network for Crystal Properties</li><li>• Distribution of Relaxation Times for Electrochemical Impedance Spectroscopy</li></ul>	
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	<b>Hong Kong University of Science and Technology</b> , Clear Water Bay, Hong Kong <i>Postdoctoral Fellow</i> Oct. 2020 - Sep. 2021 Project: Development of a Meta-solid-state Electrolyte in Li-ion Batteries <ul style="list-style-type: none"><li>• Design and develop solid-state lithium-ion batteries with a special focus on reducing the contact resistance between the electrode electrolyte interface.</li><li>• Construct deep learning models to predict the state of health for lithium-ion batteries.</li><li>• Propose graph neural networks to predict the properties of crystals and assist the high-throughput search for desired functional materials.</li></ul> <b>Hong Kong University of Science and Technology</b> , Clear Water Bay, Hong Kong <i>Ph.D. Candidate</i> Sep. 2016 - Aug. 2020	

- First-principles predictions of  $\text{Li}^+$  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  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{O}_3$ , 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  $\text{CO}_2$  Heat Pump System

- Independently carried out numerical simulations for heat transfer problems in supercritical  $\text{CO}_2$  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  $\text{CO}_2$  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  $\text{Na}_{11}\text{M}_2\text{PS}_{12}$  (M= Sn, Ge) superionic conductors. *Journal of Power Sources*, 409, 94-101. DOI: 10.1016/j.jpowsour.2018.10.077
- [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  $\text{Ba}_{0.95}\text{La}_{0.05}\text{FeO}_{3-\delta}$  as a cathode material for SOFCs. *ACS Applied Energy Materials*, 2(8), 5472-5480. DOI: 10.1021/acsaem.9b00624
- [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
- [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
- [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
- [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*. DOI: 10.1038/s41467-021-25562-y. (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)
- [9] Song, Y.<sup>†</sup>, **Liu, J.<sup>†</sup>**, 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*, 2101899. DOI: 10.1002/aenm.202101899 (co-first author)
- [10] Lin, X.<sup>†</sup>, Zhou, G.<sup>†</sup>, **Liu, J.<sup>†</sup>**, 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*, 2105717. DOI: 10.1002/adfm.202105717. (co-first author)
- [11] Zhou, M.<sup>†</sup>, **Liu, J.<sup>†</sup>**, Ye, Y., Sun, X., Chen, H., Yin, Y., Ling, Y., Ciucci F.\* and Chen, Y.\* , 2021. Enhancing the intrinsic activity and stability of perovskite cobaltite at elevated temperature through surface stress. *Small*. DOI: 10.1002/sml.202104144 (co-first author)
- [12] Wang, K.<sup>†</sup>, **Liu, J.<sup>†</sup>**, 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**)
- [13] Zhang, Z.<sup>†</sup>, **Liu, J.<sup>†</sup>**, 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)
- [14] Kim, J. H.<sup>†</sup>, Kim, J. K.<sup>†</sup>, **Liu, J.<sup>†</sup>**, 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)
- [15] 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
- [16] 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
- [17] 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
- [18] 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
- [19] Sadighi, Z., **Liu, J.**, Zhao, L., Ciucci, F., and Kim, J. K.\* , 2018. Metallic MoS<sub>2</sub> nanosheets: multifunctional electrocatalyst for the ORR, OER and Li-O<sub>2</sub> batteries. *Nanoscale*, 10(47), 22549-22559. DOI: 10.1039/C8NR07106C
- [20] Sadighi, Z., **Liu, J.**, Ciucci, F., and Kim, J. K.\* , 2018. Mesoporous MnCo<sub>2</sub>S<sub>4</sub> nanosheet arrays as an efficient catalyst for Li-O<sub>2</sub> batteries. *Nanoscale*, 10(33), 15588-15599. DOI: 10.1039/C8NR03942A
- [21] Wu, J., **Liu, J.**, Lu, Z., Lin, K., Lyu, Y. Q., Li, B., Ciucci, F.\* , and Kim, J.K.\* , 2019. Non-flammable electrolyte for dendrite-free sodium-sulfur battery. *Energy Storage Materials*, 23, 8-16. DOI: 10.1016/j.ensm.2019.05.045
- [22] 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

- [23] 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<sub>2</sub> as a high-performance sodium-ion battery anode. *Journal of Materials Chemistry A*, 8, 2114-2122. DOI: 10.1039/C9TA11913B
- [24] 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<sub>2</sub> 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
- [25] 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
- [26] 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
- [27] 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
- [28] 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
- [29] 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
- [30] Belotti, A., **Liu, J.**, Curcio, A., Wang, J., Wang, Z., Quattrocchi, E., Effat, M. B., and Ciucci, F.\* , 2021. Introducing Ag in Ba<sub>0.9</sub>La<sub>0.1</sub>FeO<sub>3-δ</sub>: combining cationic substitution with metal particles decoration. *Materials Reports: Energy*, 100018. DOI: 10.1016/j.matre.2021.100018
- [31] Wang, K., Wang, Z., Liu, Y., **Liu, J.**, Cui, Z., Zhang, X., Ciucci, F.\* , and Tang, Z.\* , 2021. Tailoring the interfacial active center of MnS<sub>x</sub>O<sub>2-x</sub>/MnCo<sub>2</sub>S<sub>4</sub> heterostructure to boost the performance for oxygen evolution reaction and Zn-Air batteries in neutral electrolyte. *Chemical Engineering Journal*. DOI: 10.1016/j.cej.2021.131966
- [32] Mamtaz, M. R. B., Wang, Z., Belotti, A., Quattrocchi, E., Yu, J., **Liu, J.**, and Ciucci, F.\* , 2021. Enhancing Ni-exsolution by nonmetal B-site substituents (Si and P) in SrTiO<sub>3</sub>-based solid oxide fuel cell anodes. *Energy & Fuels*. DOI: 10.1021/acs.energyfuels.1c01985

CONFERENCE  
ACTIVITY

**Selected poster presentations**

- [1] **Liu J.**, et al., "A theoretical study on the stability and ionic conductivity of the Na<sub>11</sub>M<sub>2</sub>PS<sub>12</sub> (M= Sn, Ge) superionic conductors", SSI-22, Jun. 2019, PyeongChang, Korea
- [2] **Liu J.**, et al., "P-substituted Ba<sub>0.95</sub>La<sub>0.05</sub>FeO<sub>3-δ</sub> as a cathode material for SOFCs", SSI-22, Jun. 2019, PyeongChang, Korea

INVITED TALKS

**Battery Modeling Webinar series**, Venkat Viswanathan, Carnegie Mellon University

Bayesian view for electrochemical impedance data Apr. 2020  
<https://pubs.acs.org/doi/full/10.1021/acsenergylett.0c01304>

PROFESSIONAL  
SERVICE

**Guest Associate Editor**

Electrochemical Energy Conversion and Storage in *Frontiers in Energy Research* Sep. 2021

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, CASTEP, Gaussian, LAMMPS, GROMACS
- Programming: Python, Matlab, C++, Pytorch, Tensorflow
- 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