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EDUCATION

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

Ph.D., Mechanical Engineering   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   Jul. 2013

RESEARCH INTERESTS

Investigating the transport phenomenon in energy materials via
- Density Functional Theory (DFT)
- Molecular Dynamics (MD)
- Finite Element Method (FEM)

Developing next-generation clean energy conversion systems, including
- Solid-State Lithium-ion Battery (SSLIB)
- Solid Oxide Fuel Cell (SOFC)
- Protonic Ceramic Fuel Cell (PCFC)

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

[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

[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.[†], **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 forReversible Protonic Ceramic Cells. ***Advanced Energy Materials***, 2101899. DOI: 10.1002/aenm.202101899 (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***, 2105717. DOI: 10.1002/adfm.202105717. (co-first author)

[11] Zhou, M.[†], **Liu, J.**[†], 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/smll.202104144 (co-first author)

[12] 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)

[13] 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)

[14] 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)

[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_2 nanosheets: multifunctional electrocatalyst for the ORR, OER and Li–O_2 batteries. ***Nanoscale***, 10(47), 22549-22559. DOI: 10.1039/C8NR07106C

[20] 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

[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_2 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. $MoSe_2$ 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

[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 $Ba_{0.9}La_{0.1}FeO_{3-\delta}$: combining cationic substitution with metal particles decoration. ***Materials Reports: Energy***, 100018. DOI: 10.1016/j.matre.2021.100018

[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 $MnS_xO_{2-x}/MnCo_2S_4$ 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 $SrTiO_3$-based solid oxide fuel cell anodes. ***Energy & Fuels***. DOI: 10.1021/acs.energyfuels.1c01985

PAPERS IN PREPARATION

[1] **Liu, J.**, Belotti, A., Kim, J. K., Koo, B., Wang, Z., Jung, W.*, and Ciucci, F.*, 2021. Understanding and mitigating A-site surface enrichment in Ba-containing perovskites: a combined computational and experimental study of $BaFeO_3$. *In submission.*

[2] **Liu, J.**, Simona, P., and Ciucci, F.*, 2021. Review of Graph Neural Networks in modeling molecules and crystal materials. *In preparation.*

[3] Simona, P., **Liu, J.**, Quattrocchi, E., and Ciucci, F.*, 2021. Neural Ordinary Differential Equations and Recurrent Neural Networks for Predicting the State of Health of Batteries. ***Journal of Energy Storage***, *In revision.* DOI: 10.26434/chemrxiv.14661180.v1

[4] Yu, J.[†], Lin, X.[†], **Liu, J.**[†] Yu, J. T., Zhou, G., Robson, M. J., Law, H. M., Kwok, S. C., Ciucci, F.*, 2021. In-Built Quasi-Solid Polymer Electrolyte for Frigostable High-Energy-Density Li-Metal Battery. *In submission.*

[5] Wang, Y.[†], Song, Y.[†], **Liu, J.**[†], Yang, K., Lin, X., Yang, Z., and Ciucci, F.[*], 2021. Functionalized Metal-supported Reversible Protonic Ceramic Cells with Exceptional Performance and Durability. *In submission.* (co-first author)

[6] Wang, Z., Wang, Y., Wang, J., Song, Y., Robson, M. J., Seong, A., Yang, M., Zhang, Z., Belotti, A., **Liu, J.**, Kim, G., Lim, J., Shao, Z., and Ciucci, F.[*], 2021. Rational design of perovskite ferrites as high-performance proton-conducting fuel cell cathodes. ***Nature Catalysis***, *In revision.*

[7] Belotti, A., Wang, Y., Curcio, A., **Liu, J.**, Quattrocchi, E., Simona, P., and Ciucci, F.[*], 2021. The influence of A-site deficiency on the electrochemical properties of $(Ba_{0.95}La_{0.05})_{1-x}FeO_{3-\delta}$ as an intermediate temperature solid oxide fuel cell cathode. ***International Journal of Hydrogen Energy***, *In submission.*

[8] Zhou, G., Yu, J., **Liu, J.**, Lin, X., Law, H. M., and Ciucci, F.[*], 2021. Quasi-solid electrolytes with tailored Li^+ solvation for fast-charging and high-power-density lithium metal batteries. ***Angewandte Chemie***, *In submission.*

CONFERENCE ACTIVITY	**Selected poster presentations** [1] **Liu J.**, et al., "A theoretical study on the stability and ionic conductivity of the $Na_{11}M_2PS_{12}$ (M= Sn, Ge) superionic conductors", SSI-22, Jun. 2019, PyeongChang, Korea [2] **Liu J.**, et al., "P-substituted $Ba_{0.95}La_{0.05}FeO_{3-\delta}$ 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)** **Ben Zhong Tang** Associate Professor Stephen K. C. Cheong Professor Dept. MAE, HKUST Dept. CHEM, HKUST E-mail: mefrank@ust.hk E-mail: tangbenz@ust.hk