YUHENG LI

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APPOINTMENT

Hong Kong University of Science and Technology, Guangzhou *2024/08 - Present*
Assistant Professor (tenure-track) & Principal Investigator

EDUCATION

University of California San Diego *2015/09 - 2020/09*
Ph.D. in NanoEngineering, Advisor: Kesong Yang

Zhejiang University *2011/09 - 2015/06*
B.E. in Materials Science and Engineering

PROFESSIONAL PREPARATION

Independent Eric and Wendy Schmidt AI in Science Fellow *2023/08 - 2024/07*
Department of Materials Science and Engineering, National University of Singapore

Postdoctoral Research Fellow *2021/01 - 2023/07*
National University of Singapore, Advisor: Pieremanuele Canepa

RESEARCH INTERESTS

- First-principles calculations, molecular dynamics
- Machine learning and high-throughput computation for data-driven materials design
- All-solid-state Li-ion and Na-ion batteries
- Hybrid halide perovskites for solar cells and light-emitting diodes
- Point defects, surface, interface, and vibrational spectroscopy
- Scientific software development

AWARDS

Eric and Wendy Schmidt AI in Science Postdoctoral Fellowship *2023/06*
Schmidt Futures, the United States

PUBLICATIONS

1. Y. Li and K. Yang, High-Throughput Computational Design of Organic–Inorganic Hybrid Halide Semiconductors Beyond Perovskites for Optoelectronics, *Energy Environ. Sci.*, 12, 2233-2243, 10.1039/C9EE01371G (2019).
2. Y. Li, P. Canepa and P. Gorai, Role of Electronic Passivation in Stabilizing the Lithium-$Li_xPO_yN_z$ Solid-Electrolyte Interphase, *PRX Energy*, 1, 023004, 10.1103/PRXEnergy.1.023004 (2022).

3. Y. Lei[#], Y. Li[#], C. Lu, Q. Yan, Y. Wu, F. Babbe, H. Gong, S. Zhang, J. Zhou, R. Wang, et al., Perovskite Superlattices with Efficient Carrier Dynamics, *Nature*, 608, 317-323, 10.1038/s41586-022-04961-1 (2022).

4. Y. Li, D. K. J. Lee, P. Cai, Z. Zhang, P. Gorai and P. Canepa, A Database of Computed Raman Spectra of Inorganic Compounds with Accurate Hybrid Functionals, *Sci. Data*, 11, 105, 10.1038/s41597-024-02924-x (2024).

5. Y. Li, A. M. Prabhu, T. S. Choksi and P. Canepa, H_2O and CO_2 Surface Contamination of the Lithium Garnet $Li_7La_3Zr_2O_{12}$ Solid Electrolyte, *J. Mater. Chem. A*, 10, 4960-4973, 10.1039/D1TA10228A (2022).

6. S. Liu[#], Y. Li[#], D. Wang[#], S. Xi, H. Xu, Y. Wang, X. Li, W. Zang, W. Liu, M. Su, et al., Alkali Cation-Induced Cathodic Corrosion in Cu Electrocatalysts, *Nature Commun.*, 15, 5080, 10.1038/s41467-024-49492-7 (2024).

7. Y. Li, D. Maldonado-Lopez, V. Ríos Vargas, J. Zhang and K. Yang, Stability Diagrams, Defect Tolerance, and Absorption Coefficients of Hybrid Halide Semiconductors: High-Throughput First-Principles Characterization, *J. Chem. Phys.*, 152, 084106, 10.1063/1.5127929 (2020).

8. Y. Li, M. Behtash, J. Wong and K. Yang, Enhancing Ferroelectric Dipole Ordering in Organic–Inorganic Hybrid Perovskite $CH_3NH_3PbI_3$: Strain and Doping Engineering, *J. Phys. Chem. C*, 122, 177-184, 10.1021/acs.jpcc.7b10413 (2018).

9. Y. Li and K. Yang, High-Throughput Computational Design of Halide Perovskites and Beyond for Optoelectronics, *WIREs Comput. Mol. Sci.*, 11, e1500, 10.1002/wcms.1500 (2021).

10. Y. Chen, Y. Lei, Y. Li, Y. Yu, J. Cai, M. Chiu, R. Rao, Y. Gu, C. Wang, W. Choi, et al., Strain Engineering and Epitaxial Stabilization of Halide Perovskites, *Nature*, 577, 209-215, 10.1038/s41586-019-1868-x (2020).

11. Y. Lei, Y. Chen, R. Zhang, Y. Li, Q. Yan, S. Lee, Y. Yu, H. Tsai, W. Choi, K. Wang, et al., A Fabrication Process for Flexible Single-Crystal Perovskite Devices, *Nature*, 583, 790-795, 10.1038/s41586-020-2526-z (2020).

12. K. Yang, Y. Li and J. Zhang, High-Throughput Screening of Hybrid Quaternary Halide Perovskites for Optoelectronics, *J. Mater. Chem. A*, 11, 6465-6473, 10.1039/D2TA09956J (2023).

13. T. Böger, T. Bernges, Y. Li, P. Canepa and W. G. Zeier, Thermal Conductivities of Lithium-Ion-Conducting Solid Electrolytes, *ACS Appl. Energy Mater.*, 6, 10704-10712, 10.1021/acsaem.3c01977 (2023).

14. H. Chen, Z. Deng, Y. Li and P. Canepa, On the Active Components in Crystalline Li–Nb–O and Li–Ta–O Coatings from First Principles, *Chem. Mater.*, 35, 5657-5670, 10.1021/acs.chemmater.3c01197 (2023).

15. A. J. K. Tieu, E. Mahayoni, Y. Li, Z. Deng, F. Fauth, J.-N. Chotard, C. Seznec, S. Adams, C. Masquelier and P. Canepa, Zirconia-Free NaSICON Solid Electrolyte Materials for Sodium All-Solid-State Batteries, *J. Mater. Chem. A*, 11, 23233-23242, 10.1039/D3TA04665F (2023).

16. B. Helm, K. Strotmann, T. Böger, B. Samanta, A. Banik, M. A. Lange, Y. Li, C. Li, M. R. Hansen, P. Canepa and W. G. Zeier, Reducing the defect formation energy by aliovalent Sn(+IV) and isovalent P(+V) substitution in Li_3SbS_4 promotes Li^+ transport, *ACS Appl. Energy Mater.*, 7, 1735-1747, 10.1021/acsaem.3c02652 (2024).

17. L. Wu, P. Lu, Y. Li, Y. Sun, J. Wong and K. Yang, First-Principles Characterization of Two-Dimensional $(CH_3(CH_2)_3NH_3)_2(CH_3NH_3)_{n-1}Ge_nI_{3n+1}$ Perovskite, *J. Mater. Chem. A*, 6, 24389-24396, 10.1039/C8TA10055A (2018).

18. Y. Li, Y. Yan, Y. Li, H. Zhang, D. Li, and D. Yang, Size-Controlled Synthesis of Pd Nanosheets for Tunable Plasmonic Properties, *CrystEngComm*, 17, 1833-1838, 10.1039/C4CE02062F (2015).

# Equal contribution

PROFESSIONAL SKILLS

- Computation: VASP, CRYSTAL, AFLOW, Lammps, Quantum Espresso
- Programming: Python, PyTorch, Pymatgen, PyLaDa, PyCDT, MongoDB

CONFERENCES

- American Physical Society (APS) March Meeting 2018, Los Angeles, Oral Presentation
- 2018 Materials Research Society (MRS) Spring Meeting & Exhibit, Phoenix, Oral Presentation
- European Materials Research Society (E-MRS) Spring Meeting 2022, online, Oral Presentation
- 2nd International Conference on Materials for Humanity (MH 22), Singapore, Oral Presentation
- 242nd Electrochemical Society (ECS) Meeting, online, Digital Presentation
- 2022 Materials Research Society (MRS) Fall Meeting & Exhibit, Boston, Oral Presentation
- 2023 Long Feng Science Forum by the Chinese University of Hong Kong, Shenzhen (CUHK-Shenzhen), online, Oral Presentation
- 2023 Inaugural Convening for the Eric and Wendy Schmidt AI in Science Postdoctoral Fellowship, Toronto, Poster Presentation
- AI for Science Summit 2023 by the Accelerate Programme at the University of Cambridge, Cambridge
- 2024 Schmidt AI in Science Regional Convening, Singapore, Oral Presentation
- International Meeting on Lithium Batteries (IMLB) 2024, Hong Kong, Poster Presentation

TEACHING

- **Guest Lecturer**: Invited Guest Lecture "Data-Driven Materials Design for Next-Generation Sustainable Energy Conversion and Storage" for the course *Sustainable Materials* (MS4667) at Nanyang Technological University (NTU) on 2023/08/30
- **Panelist**: Lecture and Discussion on "Artificial Intelligence in Materials Science" at the National University of Singapore (NUS) Roadshow on 2022/01/14
- **Mentor**: Summer programs *ENLACE* in 2017 and 2019, and *STARS* in 2017 at University of California San Diego (UCSD)
- **Teaching Assistant**: The courses *Engineering Computation Using MATLAB* (NANO/CENG 15) in Winter 2017, Winter 2018, and Fall 2019, and the course *Modeling of Nanoscale Systems* (NANO 110) in Fall 2017 at University of California San Diego (UCSD)

PEER REVIEW

Serving as a reviewer for *Nature Communications*, *The Journal of Physical Chemistry Letters*, *ACS Applied Energy Materials*, *Energy & Fuels*, *The Journal of Physical Chemistry*, and *ACS Omega*

NEWS COVERAGE

1. **May 22, 2019** "Data science helps engineers discover new materials for solar cells and LEDs" by UCSD News, UCSD Jacobs School of Engineering, Extreme Science and Engineering Discovery Environment (XSEDE), San Diego Supercomputer Center (SDSC), Phys.org, EurekAlert, etc.
2. **August 22, 2022** "Discovery offers path to safer sodium rechargeable batteries" by NUS News, TechXplore, TechNewsBoy, etc.
3. **August 10, 2022** "Perovskite material with superlattice structure might surpass efficiency of a 'perfect' solar cell" by UCSD News, UCSD Jacobs School of Engineering, etc.