

YUHENG LI

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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

WORK EXPERIENCE

Independent Eric and Wendy Schmidt AI in Science Fellow

2023/08 - Present

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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1038/s41597-024-02924-x) (2024).

5. Y. Li, A. M. Prabhu, T. S. Choksi and P. Canepa, H₂O and CO₂ Surface Contamination of the Lithium Garnet Li₇La₃Zr₂O₁₂ Solid Electrolyte, *J. Mater. Chem. A*, 10, 4960-4973, [10.1039/D1TA10228A](#) (2022).
6. 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).
7. Y. Li, M. Behtash, J. Wong and K. Yang, Enhancing Ferroelectric Dipole Ordering in Organic–Inorganic Hybrid Perovskite CH₃NH₃PbI₃: Strain and Doping Engineering, *J. Phys. Chem. C*, 122, 177-184, [10.1021/acs.jpcc.7b10413](#) (2018).
8. 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).
9. 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).
10. 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).
11. 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).
12. 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).
13. 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).
14. 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).
15. 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 Li₃SbS₄ promotes Li⁺ transport, *ACS Appl. Energy Mater.*, x, xx-xx, [xxx](#) (2024).
16. L. Wu, P. Lu, Y. Li, Y. Sun, J. Wong and K. Yang, First-Principles Characterization of Two-Dimensional (CH₃(CH₂)₃NH₃)₂(CH₃NH₃)_{n-1}Ge_nI_{3n+1} Perovskite, *J. Mater. Chem. A*, 6, 24389-24396, [10.1039/C8TA10055A](#) (2018).
17. 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 (IMLB) 2024

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* ([link](#)), *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.