

Zhenglu Li

Assistant Professor

Mork Family Department of Chemical Engineering and Materials Science

Viterbi School of Engineering \diamond University of Southern California

CONTACT

Address: VHE 508, Vivian Hall of Engineering, 3651 Watt Way, Los Angeles, CA 90089

Email: zhenglul@usc.edu

Website: sites.usc.edu/ligroup

EMPLOYMENT

Assistant Professor

January 2023 - Present

Mork Family Department of Chemical Engineering and Materials Science

Viterbi School of Engineering, University of Southern California

- Computational Quantum Materials Group ([link](#))

Postdoctoral Researcher

August 2019 - December 2022

Lawrence Berkeley National Laboratory & University of California at Berkeley

Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPPEM)

- Advisor: Prof. Steven G. Louie

Research Assistant

July 2012 - July 2013

Department of Physics, Fudan University

- Advisor: Prof. Xingao Gong and Prof. Hongjun Xiang

EDUCATION

Ph.D. in Physics, University of California at Berkeley

August 2013 - August 2019

- Advisor: Prof. Steven G. Louie
- Thesis: Electron-phonon coupling from *GW* perturbation theory and electronic and magnetic properties of novel two-dimensional materials (*APS Metropolis Award*)

B.S. in Physics, Fudan University

September 2008 - July 2012

- Advisor: Prof. Xingao Gong and Prof. Hongjun Xiang
- Thesis: First-principles studies of topological insulators and multiferroics

RESEARCH INTERESTS

- Developments and applications of *ab initio* many-body computational methods for quantum excited states and dynamics.
- Electron-phonon coupling and its interplay with many-electron correlation in oxide superconductors, flat-band materials, and heterostructures.
- Exotic electron and exciton phases in two-dimensional moiré superlattices, such as Wigner crystals and correlated moiré excitons.
- Nonequilibrium exciton-phonon coupled dynamics, coherence in energy transfer processes, and simulations of pump-probe ultrafast spectroscopies.

HONORS AND AWARDS

- **NSF CAREER Award, PI**, 2025. ([link](#))
- **DOE INCITE Award, PI** (Co-PI: Mauro Del Ben), *Exascale Simulation of Correlated Electron-Phonon Coupling in Quantum Materials*, granted 1,000,000 GPU node hours (total) over two years, 1/2024 - 12/2025. ([link](#))
- **APS Nicholas Metropolis Award** for Outstanding Doctoral Thesis Work in Computational Physics, American Physical Society, 2021. ([link](#))
- **ACM Gordon Bell Prize Finalist, Team**, Association for Computing Machinery, 2020.
- **Allan and Kathleen Rosevear Gateway Fellowship**, International House & Graduate Division, University of California at Berkeley, 2013.
- **Undergraduate Thesis Award**, Department of Physics, Fudan University, 2012.

TEACHING

- **MASC 110L: Materials Science**, University of Southern California, Fall 2023 and Fall 2024.
- **MASC 520: Mathematical Methods for Deep Learning**, University of Southern California, Spring 2024.

PUBLICATIONS

- Total **6,400+** citations and h-index of **20** from Google Scholar (Last update: January 28, 2025) ([link](#)).
- Publications include **2** Nature, **1** Science, **2** Nature Materials, **7** Phys. Rev. Lett., **5** Nano Lett., **3** Proc. Natl. Acad. Sci., **2** Nature Commun., among others.

(* denotes corresponding authorship; † denotes equal contributions; **SELECTED** publications indicated)

36. J.-Y. You, C.-E. Hsu, M. Del Ben, and **Z. Li***, *Diverse manifestations of electron-phonon coupling in a kagome superconductor*, arXiv:2411.07427, Phys. Rev. Lett., *accepted* (2025). [DOI](#) **SELECTED**
35. J.-Y. You, Z. Zhu, M. Del Ben, W. Chen, and **Z. Li***, *Unlikelihood of a phonon mechanism for the high-temperature superconductivity in $La_3Ni_2O_7$* , npj Comput. Mater. **11**, 3 (2025). [DOI](#)
34. Y.-H. Chan, **Z. Li**, and S. G. Louie, *Excitonic effects on infrared vibrational and Raman spectroscopy from first principles*, arXiv:2412.16439 (2024). [DOI](#)
33. W. Lee, A. M. Alvertis, **Z. Li**, S. G. Louie, M. R. Filip, J. B. Neaton, and E. Kioupakis, *Phonon screening of excitons in atomically thin semiconductors*, Phys. Rev. Lett. **133**, 206901 (2024). [DOI](#)
32. **Z. Li** and S. G. Louie, *Two-gap superconductivity and decisive role of rare-earth d electrons in infinite-layer nickelates*, Phys. Rev. Lett. **133**, 126401 (2024). [DOI](#) (Editors' Suggestion) **SELECTED**
31. A. M. Alvertis, J. B. Haber, **Z. Li**, C. J. N. Coveney, S. G. Louie, M. R. Filip, and J. B. Neaton, *Phonon screening and dissociation of excitons at finite temperatures from first principles*, Proc. Natl. Acad. Sci. **121**, e2403434121 (2024). [DOI](#)
30. H. Li, Z. Xiang, M. H. Naik, W. Kim, **Z. Li**, R. Sailus, R. Banerjee, T. Taniguchi, K. Watanabe, S. Tongay, A. Zettl, F. H. da Jornada, S. G. Louie, M. F. Crommie, and F. Wang, *Imaging moiré excited states with photocurrent tunneling microscopy*, Nature Mater. **23**, 633 (2024). [DOI](#)
29. **Z. Li**, G. Antonius, Y.-H. Chan, and S. G. Louie, *Electron-phonon coupling from GW perturbation theory: Practical workflow combining BerkeleyGW, ABINIT, and EPW*, Comput. Phys. Commun. **295**, 109003 (2024). [DOI](#)

28. H. Wang, Y. Zhong, W. Jiang, S. Latini, S. Xia, T. Cui, **Z. Li**, T. Low, and F. Liu, *Strain-Tunable Hyperbolic Exciton Polaritons in Monolayer Black Arsenic with Two Exciton Resonances*, Nano Lett. **24**, 2057 (2024). [DOI](#)
27. C. Chen, W. Tang, X. Chen, Z. Kang, S. Ding, K. Scott, S. Wang, **Z. Li**, J. P. C. Ruff, M. Hashimoto, D.-H. Lu, C. Jozwiak, A. Bostwick, E. Rotenberg, E. H. Neto, R. J. Birgeneau, Y. Chen, S. G. Louie, Y. Wang, and Y. He, *Anomalous excitonic phase diagram in band-gap-tuned $Ta_2Ni(Se,S)_5$* , Nature Commun. **14**, 7512 (2023). [DOI](#)
26. C. Chen, X. Chen, W. Tang, **Z. Li**, S. Wang, C. Jozwiak, A. Bostwick, E. Rotenberg, M. Hashimoto, D. Lu, J. P. C. Ruff, S. G. Louie, R. Birgeneau, Y. Chen, Y. Wang, and Y. He, *Lattice fluctuation induced pseudogap in quasi-one-dimensional Ta_2NiSe_5* , Phys. Rev. Research **5**, 043089 (2023). [DOI](#)
25. J. Ruan, **Z. Li**, C. S. Ong, and S. G. Louie, *Two-dimensional single-valley exciton qubit and optical spin magnetization generation*, Proc. Natl. Acad. Sci. **120**, e2307611120 (2023). [DOI](#)
24. M. H. Naik, E. C. Regan, Z. Zhang, Y. Chan, **Z. Li**, D. Wang, Y. Yoon, C. S. Ong, W. Zhao, S. Zhao, M. I. B. Utama, B. Gao, X. Wei, M. Sayyad, K. Yumigeta, K. Watanabe, T. Taniguchi, S. Tongay, F. H. da Jornada, F. Wang and S. G. Louie, *Intralayer charge-transfer moiré excitons in van der Waals superlattices*, Nature **609**, 52 (2022). [DOI](#)
23. Y. Lin, Y.-H. Chan, W. Lee, L.-S. Lu, **Z. Li**, W.-H. Chang, C.-K. Shih, R. A. Kaindl, S. G. Louie, and A. Lanzara, *Exciton-driven renormalization of quasiparticle band structure in monolayer MoS_2* , Phys. Rev. B **106**, L081117 (2022). [DOI](#)
22. F. Tang, **Z. Li**, C. Zhang, S. G. Louie, R. Car, D. Y. Qiu, and X. Wu, *Many-body effects in the X-ray absorption spectra of liquid water*, Proc. Natl. Acad. Sci. **119**, e2201258119 (2022). [DOI](#)
21. T. Chagas, O. A. Ashour, G. A. S. Ribeiro, W. S. Silva, **Z. Li**, S. G. Louie, R. Magalhaes-Paniago, and Y. Petroff, *Multiple strong topological gaps and hexagonal warping in Bi_4Te_3* , Phys. Rev. B **105**, L081409 (2022). [DOI](#)
20. M. Wu, **Z. Li**, and S. G. Louie, *Optical and magneto-optical properties of ferromagnetic monolayer $CrBr_3$: A first-principles GW and GW plus Bethe-Salpeter equation study*, Phys. Rev. Mater. **6**, 014008 (2022). [DOI](#)
19. S. G. Louie, Y.-H. Chan, F. H. da Jornada, **Z. Li**, and D. Y. Qiu, *Discovering and understanding materials through computation*, Nature Materials **20**, 728 (2021). [DOI](#) (Invited Perspective for Insight Issue *Computational Materials Design*) **SELECTED**
18. **Z. Li**, M. Wu, Y.-H. Chan, and S. G. Louie, *Unmasking the origin of kinks in the photoemission spectra of cuprate superconductors*, Phys. Rev. Lett. **126**, 146401 (2021). [DOI](#) (Editors' Suggestion) **SELECTED**
News: [OLCF](#), [TACC](#).
17. X. Jiang, C. Shi, **Z. Li**, S. Wang, Y. Wang, S. Yang, S. G. Louie, and X. Zhang, *Direct observation of Klein tunneling in phononic crystals*, Science **370**, 1447 (2020). [DOI](#)
16. M. Del Ben, C. Yang, **Z. Li**, F. H. da Jornada, S. G. Louie, and J. Deslippe, *Accelerating large-scale excited-state GW calculations on leadership class HPC systems*, SC20: International Conference for High Performance Computing, Networking, Storage and Analysis **1**, 36 (2020). [DOI](#) (ACM Gordon Bell Prize Finalist) **SELECTED**
News: [OLCF](#).
15. E. Gaufrès, F. Fossard, V. Gosselin, L. Sponza, F. Ducastelle, **Z. Li**, S. G. Louie, R. Martel, M. Côté, and A. Loiseau, *Momentum-resolved dielectric response of free-standing mono-, bi-, and trilayer black phosphorus*, Nano Lett. **19**, 8303 (2019). [DOI](#)

14. M. Wu, **Z. Li**, T. Cao, and S. G. Louie, *Physical origin of giant excitonic and magneto-optical responses in two-dimensional ferromagnetic insulators*, Nature Commun. **10**, 2371 (2019). [DOI](#)
13. **Z. Li**, G. Antonius, M. Wu, F. H. da Jornada, and S. G. Louie, *Electron-phonon coupling from ab initio linear-response theory within the GW method: Correlation-enhanced interactions and superconductivity in $Ba_{1-x}K_xBiO_3$* , Phys. Rev. Lett. **112**, 186402 (2019). [DOI](#) **SELECTED**
12. **Z. Li**, T. Cao, and S. G. Louie, *Two-dimensional ferromagnetism in few-layer van der Waals crystals: Renormalized spin-wave theory and calculations*, J. Mag. Mag. Mat. **463**, 28 (2018). [DOI](#) (Invited contribution to *Special Issue in Memory of A. J. Freeman*)
11. K. Gotlieb[†], **Z. Li**[†], C.-Y. Lin, C. Jozwiak, J. H. Ryoo, C.-H. Park, Z. Hussain, S. G. Louie, and A. Lanzara, *Symmetry rules shaping spin-orbital textures in surface states*, Phys. Rev. B **95**, 245142 (2017). [DOI](#)
10. C. Gong[†], L. Li[†], **Z. Li**[†], H. Ji, A. Stern, Y. Xia, T. Cao, W. Bao, C. Wang, Y. Wang, Z. Q. Qiu, R. J. Cava, S. G. Louie, J. Xia, and X. Zhang, *Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals*, Nature **546**, 265 (2017). [DOI](#) **SELECTED**
News: [Nature News](#), [Physics Today](#), [LBNL News](#).
9. **Z. Li**, T. Cao, M. Wu, and S. G. Louie, *Generation of anisotropic massless Dirac fermions and asymmetric Klein tunneling in few-layer black phosphorus superlattices*, Nano Lett. **17**, 2280 (2017). [DOI](#) **SELECTED**
8. T. Helm, F. Flicker, R. Kealhofer, P. J. W. Moll, I. M. Hayes, N. P. Breznay, **Z. Li**, S. G. Louie, Q. R. Zhang, L. Balicas, J. E. Moore, and J. G. Analytis, *Thermodynamic anomaly above the superconducting critical temperature in the quasi-one-dimensional superconductor $Ta_4Pd_3Te_{16}$* , Phys. Rev. B **95**, 075121 (2017). [DOI](#)
7. T. Pham, A. L. Gibb, **Z. Li**, S. M. Gilbert, C. Song, S. G. Louie, and A. Zettl, *Formation and dynamics of electron-irradiation-induced defects in hexagonal boron nitride at elevated temperatures*, Nano Lett. **16**, 7142 (2016). [DOI](#)
6. T. Cao, **Z. Li**, D. Y. Qiu, and S. G. Louie, *Gate switchable transport and optical anisotropy in 90° twisted bilayer black phosphorus*, Nano Lett. **16**, 5542 (2016). [DOI](#)
5. T. Cao, **Z. Li**, and S. G. Louie, *Tunable magnetism and half-metallicity in hole-doped monolayer GaSe*, Phys. Rev. Lett. **114**, 236602 (2015). [DOI](#)
4. **Z. Li**[†], Z.-M. Li[†], H.-Y. Cao, J.-H. Yang, Q. Shu, Y.-Y. Zhang, H. J. Xiang, and X. G. Gong, *What are grain boundary structures in graphene?*, Nanoscale **6**, 4309 (2014). [DOI](#)
3. **Z. Li**, M.-H. Whangbo, X. G. Gong, and H. J. Xiang, *Helicoidal magnetic structure and ferroelectric polarization in $Cu_3Nb_2O_8$* , Phys. Rev. B **86**, 174401 (2012). [DOI](#)
2. J.-H. Yang, **Z. Li**, X. Z. Lu, M.-H. Whangbo, S.-H. Wei, X. G. Gong, and H. J. Xiang, *Strong Dzyaloshinskii-Moriya interaction and origin of ferroelectricity in Cu_2OSeO_3* , Phys. Rev. Lett. **109**, 107203 (2012). [DOI](#)
1. **Z. Li**, J. H. Yang, G. H. Chen, M.-H. Whangbo, H. J. Xiang, and X. G. Gong, *Strong single-ion anisotropy and anisotropic interactions of magnetic adatoms induced by topological surface states*, Phys. Rev. B **85**, 054426 (2012). [DOI](#)

INVITED TALKS

- CECAM Workshop - Recent advances in first-principles modeling of electron-phonon interactions, Lausanne, Switzerland, December 2025 (upcoming).

- Materials Science and Engineering Colloquium, Department of Applied Physics and Applied Mathematics, Columbia University, New York, November 2024.
- CECAM and Psi-k Workshop - Frontiers in many-body excited-state dynamics from first principles, Lausanne, Switzerland, July 2024.
- CIMTEC 2024 - Global Conference “Materials in an Explosively Growing Informatics World”, Montecatini Terme, Italy, June 2024.
- Seminar, Department of Physics, University of California at Santa Cruz, Santa Cruz, May 2024.
- APS March Meeting, Minneapolis, March 2024.
- Solid State Seminar, Department of Applied Physics, Yale University, New Haven, November 2023.
- Condensed Matter Physics Seminar, Department of Physics, University of Texas at Austin, Austin, October 2023.
- Seminar, Oden Institute, University of Texas at Austin, Austin, October 2023.
- 9th International Conference on Energy, Materials, and Photonics (EMP23), National University of Singapore, Singapore, August 2023.
- Conference of Condensed Matter Physics, Liyang, China, August 2023.
- Joint USA-European Symposium on Extreme-Scale Simulations, Machine Learning, and Neutron & X-Ray Scattering for Quantum Materials, Spetses, Greece, July 2023.
- Seminar, Department of Physics, Southern University of Science and Technology (SUSTech), Shenzhen, China, May 2023.
- Seminar, Laboratory of Computational Physical Sciences, Fudan University, Shanghai, China, May 2023.
- Seminar, Department of Physics, Shanghai Jiao Tong University, Shanghai, China, May 2023.
- TMS Annual Meeting & Exhibition, Computational Thermodynamics and Kinetics Symposium, San Diego, March 2023.
- Condensed Matter Seminar (290K), Department of Physics, University of California at Berkeley, Berkeley, October 2022.
- Seminar (online), Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, February 2022.
- Seminar, Department of Mechanical Engineering, University of Rochester, Rochester, February 2022.
- Excited States Mini-Workshop (online), National Center for Theoretical Sciences, Physics Division, Taiwan, February 2022.
- Seminar, Mork Family Department of Chemical Engineering and Materials Science, University of Southern California, Los Angeles, February 2022.
- Condensed Matter Seminar, Department of Physics, University of California at Davis, Davis, October 2021.
- Workshop on Recent Developments in Electronic Structure Methods (online), Flatiron Institute, New York, July 2021.
- APS March Meeting (online), APS Nicholas Metropolis Award talk, March 2021.
- Condensed Matter Physics Seminar (online), Department of Physics, Washington University in St. Louis, November 2020.
- ABC Physics Seminar, Department of Physics, University of Washington, Seattle, February 2020.
- Berkeley Excited States Conference, Oakland, June 2019.

SERVICE AND OUTREACH

- Co-organizer and instructor of *School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows*, 2022 - present. ([link](#))
- Co-organizer of *Berkeley Excited States Conference (BESC)*, 2021 - present. ([link](#))
- Co-organizer and instructor of the *Annual BerkeleyGW Tutorial Workshop*, 2015 - present. ([link](#))

- Main developer of the open-source BerkeleyGW software package, 2015 - present.
- Co-chair for *Frontiers in Condensed Matter and Materials Physics: A Symposium in Honor of the 75th Birthday of Steven G. Louie*, Berkeley, 2024. ([link](#))
- Reviewer for Leibniz Competition, Leibniz Association, Berlin, Germany, 2023. ([link](#))
- Member of the Selection Committee for the *APS Nicholas Metropolis Award*, 2022. ([link](#))
- Organizing committee member of *Frontiers in Condensed Matter and Materials Physics: A Scientific Symposium in Honor of the 70th Birthday of Steven G. Louie*, 2019. ([link](#))
- Reviewer for *PRL*, *Nat. Rev. Phys.*, *Nat. Commun.*, *Nano Lett.*, *npj Comput. Mat.*, *Adv. Mater.*, *PRB*, among others.
- *Summer High School Intensive in Next-Generation Engineering (SHINE) Program*, providing research experiences to high-school students, Viterbi School of Engineering, University of Southern California, 2023 - present. ([link](#))
- *Viterbi Summer Institute (VSI) Program*, a high achievement program designed to enhance the transition to college for engineering students from underrepresented backgrounds, Viterbi School of Engineering, University of Southern California, 2024 - present. ([link](#))
- *Summer Undergraduate Research Experience (SURE) Program*, summer residential research program for external undergraduate students, Viterbi School of Engineering, University of Southern California, 2024 - present. ([link](#))