

Zhenglu Li

Assistant Professor

Mork Family Department of Chemical Engineering and Materials Science
Viterbi School of Engineering ◊ University of Southern California

CONTACT

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EMPLOYMENT

Assistant Professor *January 2023 -*
Mork Family Department of Chemical Engineering and Materials Science
Viterbi School of Engineering, University of Southern California

- Computational Quantum Materials Research 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 (C2SEPEM)

- 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

- Development and application of *ab initio* many-body computational methods for quantum excitations and dynamics.
- Electron-phonon coupling and its interplay with many-electron correlation in high- T_c superconductors and flat-band materials and two-dimensional atomically thin layers.
- Nonequilibrium exciton dynamics involving electronic and vibrational coherence in energy materials and devices.
- Manipulation of quantum electronic, excitonic, and magnetic excitations in two-dimensional materials and solid-state qubits.

HONORS AND AWARDS

- **APS Nicholas Metropolis Award** for Outstanding Doctoral Thesis Work in Computational Physics, American Physical Society, 2021. ([link](#))
- **ACM Gordon Bell Prize Finalist**, Association for Computing Machinery, 2020. ([link](#))
- **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.

PUBLICATIONS

*In reverse chronological order; * denotes equal contribution; **SELECTED** publications indicated.*

27. J. Ruan, **Z. Li**, C. S. Ong, and S. G. Louie, *Two-dimensional single-valley exciton qubit and optical spin magnetization generation*, arXiv:2211.03334 (2022).
26. **Z. Li** and S. G. Louie, *Two-gap superconductivity and decisive role of rare-earth d electrons in infinite-layer nickelates*, arXiv:2210.12819 (2022). **SELECTED**
25. 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 Ta₂NiSe₅*, arXiv:2203.06817 (2022).
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 MoS₂*, 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 Bi₄Te₃*, Phys. Rev. B **105**, L081409 (2022). [DOI](#)
20. M. Wu, **Z. Li**, and S. G. Louie, *Optical and magneto-optical properties of ferromagnetic monolayer CrBr₃: 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.

INVITED TALKS

- TMS Annual Meeting & Exhibition, Computational Thermodynamics and Kinetics Symposium, San Diego, March 2023 (invited).
- Condensed Matter Seminar (290K), Department of Physics, University of California at Berkeley, October 2022.
- Seminar (online), Department of Materials Science and Engineering, University of Wisconsin-Madison, February 2022.
- Seminar, Department of Mechanical Engineering, University of 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, February 2022.
- Condensed Matter Seminar, Department of Physics, University of California at 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.
- Seminar, Laboratory for Computational Physical Sciences, Fudan University, Shanghai, April 2018.

SERVICE

- Organizing committee member of *Berkeley Excited States Conference (BESC)*, 2021 - present. ([link](#))
- Co-organizer and Instructor of the *Annual BerkeleyGW Tutorial Workshop*, 2014 - present. ([link](#))
- Selection committee member for the APS Nicholas Metropolis Award, 2022. ([link](#))
- Reviewer for *PRL*, *Nature Commun.*, *Nano Lett.*, *npj Comput. Mat.*, *Adv. Mater.*, *PRB*, among others.