Xiaoxiong Liu

Curriculum Vitae

General

Born 2nd Feb 1993

Nationality China

E-mail xxliu@physik.uzh.ch

Position Ph.D. student in condensed matter physics, University of Zurich, Switzerland

Education

2019–present **Ph.D. in Condensed Matter Physics**, *University of Zurich*, Switzerland.
Supervisor: Dr. Stepan S. Tsirkin

2016–2019 **M.Sc. in Theoretical Physics**, *Lanzhou University*, China.
Thesis: Electronic Properties Study of Topological Weyl Semimetals in Space Group $F\bar{4}3m$.
Supervisor: Prof. Jianbo Deng

2012–2016 **B.Sc. in Physics**, *Lanzhou University*, China.
Thesis: First-principle investigations of 3d transition metal (Fe, Cu, and Co)-doped rocksalt MgO by chain. Supervisor: Prof. Jianbo Deng

Teaching Assistant

University of Zurich

2022 Quantum Mechanics

2022 Machine Learning for the Sciences

2021 Mathematical Methods of Physics I

2021 Linear Algebra II

2020 Linear Algebra I

2020 Scientific Computing

Lanzhou University

2016 Mechanics

Awards

2018 National Scholarship of Graduated Student.

Languages

Chinese **Native**

English **Professional Fluency**

Find Me on Web

HomePage https://liu-xiaoxiong.github.io/index.html

GroupPage https://www.physik.uzh.ch/en/groups/neupert/team/Xiaoxiong-Liu.html

Scholar https://scholar.google.com/citations?user=s2Py778AAAAJ&hl=zh-CN&oi=ao

ResearchGate https://www.researchgate.net/profile/Xiaoxiong-Liu

Github https://github.com/Liu-Xiaoxiong

Gitlab https://gitlab.com/Xiaoxiong_Liu

Development of Scientific Software (open source)

Author of:

symmetrize wann matrix — This code aimed to symmetrize matrix elements from Wannier90. E.g., Hamiltonian and position elements.

Code available at: https://github.com/Liu-Xiaoxiong/symmetrize_wann_matrix

Main Developer of:

WannierBerri — An advanced tool for Wannier interpolation and integration of quantities related to Berry curvature and magnetic moment. http://wannier-berri.org

Code available at: https://github.com/wannier-berri/wannier-berri

Contributor of: (in progress)

ASE — The Atomic Simulation Environment (ASE) is a set of tools and Python modules for setting up, manipulating, running, visualizing, and analyzing atomistic simulations. I am improving the Wannier function part of ASE. https://wiki.fysik.dtu.dk/ase/

Computer Skills

Programing	*Python3, Fortran, Mathematica, Linux*
DFT code	*VASP, QuantumEspresso,FPLO,Abnit,Siesta,ASE*
Post-DFT	*Wannier90,WannierBerri,WannierTools,Irrep,Z2Pack*
High-Throughput	*AiiDA*

Publication Activity

15 Publications, including: Nature Material(1), Communications Physics(1), PRL(1), PRB(2), APL(1)

279 citations.

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References

Group Leader **Titus Neupert**, Institut-Physik, University of Zurich, <neupert@physik.uzh.ch>.

Supervisor **Stepan S Tsirkin**, Institut-Physik, University of Zurich, <stepan@physik.uzh.ch>.

co-author **Ivo Souza**, CMF, University of the Basque Country, <ivo_souza@ehu.eus> >.

Participation in Conferences

Oral Contributions

2. Symmetrization of berry curvature and magnetic moment, **Wannier 2022 Developers Meeting (smr 3757)**, ICTP, Trieste, Italy, May 23-27, 2022

1. Gauge-covariant derivatives of the Berry curvature and orbital moment by Wannier interpolation, **APS March meeting**, Virtual, USA, March 15-19, 2021

Poster Contributions

8. Ab initio calculations of electrical magnetochiral anisotropy with Wannier interpolation, **Swiss Workshop on Materials with Novel Electronic Properties Basic research and applications**, Les Diablerets, Switzerland, August 29-31, 2022

7. Ab initio calculations of electrical magnetochiral anisotropy with Wannier interpolation, **Psi-K Conference**, EPFL, Lausanne, Switzerland, August 22-25, 2022

6. Systematic study of magnetotransport responses with Berry-Boltzmann formalism, **First-Principles Modelling of Defects in Solids Workshop**, ETHz, Zurich, Switzerland, June 13-15, 2022

5. Systematic study of magnetotransport responses with Berry-Boltzmann formalism, **Wannier 2022 Summer School**, ICTP, Trieste, Italy May 16-20, 2022

4. Wannier Interpolation of Berry-Boltzmann Formalism for Berry Curvature related quantities with WannierBerri, **Condensed Matter Theory Symposium**, ETHz, Zurich, Switzerland, September 22, 2021

3. Gauge-covariant derivatives of the Berry curvature and orbital moment by Wannier interpolation, **Virtual DPG Spring Meeting**, Virtual, Germany, March 1-4, 2021

2. Gauge-covariant derivatives of the Berry curvature and orbital moment by Wannier interpolation, **20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**, Virtual, Italy, February 23-25, 2021

1. Gauge-covariant derivatives of the Berry curvature and orbital moment by Wannier interpolation, **Virtual Electronic Structure Workshop**, Virtual, USA, June 3-5, 2020

Publications

18. Ab initio calculations of electrical magnetochiral anisotropy with Wannier interpolation, Xiaoxiong Liu, S. S. Tsirkin, I. Souza, in progress.

17. Systematic study of magnetotransport responses with Berry-Boltzmann formalism, Xiaoxiong Liu, S. S. Tsirkin, I. Souza, in progress.

16. Covariant derivatives of Berry-type quantities: Application to nonlinear transport,Xiaoxiong Liu, M. Á. Jiménez, S. S. Tsirkin, I. Souza, in progress.

15. Two-dimensional sliding charge density waves and their protected edge modes, SB Zhang, MS Hossain, JX Yin, Xiaoxiong Liu, MZ Hasan, T Neupert, arXiv preprint arXiv:2204.06269

14. Origin of spin reorientation and intrinsic anomalous Hall effect in the kagome ferrimagnet TbMn6Sn6, DC Jones, S Das, H Bhandari, Xiaoxiong Liu, P Siegfried, MP Ghimire, SS Tsirkin, II Mazin, NJ Ghimire, arXiv e-prints, arXiv: 2203.17246

13. Triple nodal points characterized by their nodal-line structure in all magnetic space groups, PM Lenggenhager, Xiaoxiong Liu, T Neupert, T Bzdušek, arXiv preprint arXiv:2201.08404

12. Intriguing magnetism of the topological kagome magnet $TbMn_6Sn_6$, C Mielke III, Wenlong Ma, V Pomjakushin, O Zaharko, Xiaoxiong Liu, J-X Yin, SS Tsirkin, TA Cochran, M Medarde, V Poree, D Das, CN Wang, J Chang, T Neupert, A Amato, S Jia, MZ Hasan, H Luetkens, Z Guguchia, Communications Physics 5 (1), 1-9 (2022)

11. Signatures of Weyl fermion annihilation in a correlated kagome magnet, I. Belopolski, T. A. Cochran, Xiaoxiong Liu, Z. Cheng, X. Yang, Z. Guguchia, S. S. Tsirkin, J. Yin, P. Vir, G. S. Thakur, S. Zhang, J. Zhang, K. Kaznatcheev, G. Cheng, G. Chang, D. Multer, N. Shumiya, M. Litskevich, E. Vescovo, T. K. Kim, C. Cacho, N. Yao, C. Felser, T. Neupert, M. Z. Hasan, **Physical review letters** 127 (25), 256403, (2021)

10. Unconventional chiral charge order in kagome superconductor KV3Sb5, Y. Jiang, J. Yin, M. M. Denner, N. Shumiya, B. R. Ortiz, G. Xu, Z. Guguchia, J. He, M. S. Hossain, Xiaoxiong Liu, J. Ruff, L. Kautzsch, S. Zhang, G. Chang, I. Belopolski, Q. Zhang, T. A. Cochran, D. Multer, M. Litskevich, Z. Cheng, X. Yang, Z. Wang, R. Thomale, T. Neupert, S. D. Wilson, M. Z. Hasan, **Nature Materials** 20 (10), 1353-1357, (2021)

9. Universal higher-order bulk-boundary correspondence of triple nodal points, PM Lenggenhager, Xiaoxiong Liu, T Neupert, T Bzdušek, arXiv preprint arXiv:2104.11254

8. From triple-point materials to multiband nodal links, PM Lenggenhager, Xiaoxiong Liu, SS Tsirkin, T Neupert, T Bzdušek, **Physical Review B** 103 (12), L121101, (2021)

7. Magneto-transport and Shubnikov–de Haas oscillations in the type–II Weyl semimetal candidate NbIrTe4 flake, X. Huang, Xiaoxiong Liu, P. Yu, P. Li, J. Cui, J. Yi, J. Deng, J. Fan, Z. Ji, F. Qu, X. Jing, C. Yang, L Lu, Z. Liu, G. Liu, **Chinese Physics Letters** 36 (7), 077101, (2019)

6. Quantum anomalous Hall effect and topological phase transition in two-dimensional antiferromagnetic Chern insulator NiOsCl6, WW Yang, L Li, JS Zhao, Xiaoxiong Liu, JB Deng, XM Tao, XR Hu, **Journal of Physics: Condensed Matter** 30 (18), 185501, (2018)

5. A nonmagnetic topological Weyl semimetal in quaternary Heusler compound CrAlTiV, Xiaoxiong Liu, L Li, Y Cui, J Deng, X Tao, **Applied Physics Letters** 111 (12), 122104, (2017)

4. Ternary Weyl semimetal $NbIrTe_4$ proposed from first-principles calculation, L Li, HH Xie, JS Zhao, Xiaoxiong Liu, JB Deng, XR Hu, XM Tao, **Physical Review B** 96 (2), 024106, (2017)

3. First-principle investigations of 3d transition metal (Fe, Cu, and Co)-doped rocksalt MgO by chain, Xiaoxiong Liu, Q Gao, L Li, J Zhao, X Hu, J Deng, **Journal of Superconductivity and Novel Magnetism** 30 (6), 1635-1641, (2017)

2. Effect of As and Nb doping on the magnetic properties for quaternary Heusler alloy FeCoZrGe, GY Mao, Xiaoxiong Liu, Q Gao, L Li, HH Xie, G Lei, JB Deng, **Journal of Magnetism and Magnetic Materials** 398, 1-6, (2016)

1. First-principle study of half-metallic ferromagnetism in rocksalt XO (X= Li, K, Rb, Cs), G Lei, Xiaoxiong Liu, HH Xie, L Li, Q Gao, JB Deng,**Journal of Magnetism and Magnetic Materials** 397, 176-180, (2016)