



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	<i>Python3, Fortran, Mathematica, Linux</i>
DFT code	<i>VASP, QuantumEspresso, FPLO, Abnit, Siesta, ASE</i>
Post-DFT	<i>Wannier90, WannierBerri, WannierTools, Irrep, Z2Pack</i>
High-Throughput	<i>AiiDA</i>

Publication Activity

15 Publications, including: Nature Material(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

1. Symmetrization of berry curvature and magnetic moment, **Wannier 2022 Developers Meeting (smr 3757)**, ICTP, Trieste, Italy, May 23-27, 2022
2. Gauge-covariant derivatives of the Berry curvature and orbital moment by Wannier interpolation, **APS March meeting**, Virtual, USA, March 15-19, 2021

Poster Contributions

1. 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
2. Ab initio calculations of electrical magnetochiral anisotropy with Wannier interpolation, **Psi-K Conference**, EPFL, Lausanne, Switzerland, August 22-25, 2022
3. Systematic study of magnetotransport responses with Berry-Boltzmann formalism, **First-Principles Modelling of Defects in Solids Workshop**, ETHz, Zurich, Switzerland, June 13-15, 2022
4. Systematic study of magnetotransport responses with Berry-Boltzmann formalism, **Wannier 2022 Summer School**, ICTP, Trieste, Italy May 16-20, 2022
5. Wannier Interpolation of Berry-Boltzmann Formalism for Berry Curvature related quantities with WannierBerri, **Condensed Matter Theory Symposium**, ETHz, Zurich, Switzerland, September 22, 2021
6. Gauge-covariant derivatives of the Berry curvature and orbital moment by Wannier interpolation, **Virtual DPG Spring Meeting**, Virtual, Germany, March 1-4, 2021
7. 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
8. Gauge-covariant derivatives of the Berry curvature and orbital moment by Wannier interpolation, **Virtual Electronic Structure Workshop**, Virtual, USA, June 3-5, 2020

Publications

1. Ab initio calculations of electrical magnetochiral anisotropy with Wannier interpolation, [Xiaoxiong Liu](#), S. S. Tsirkin, I. Souza, in progress.
2. Systematic study of magnetotransport responses with Berry-Boltzmann formalism, [Xiaoxiong Liu](#), S. S. Tsirkin, I. Souza, in progress.

3. Covariant derivatives of Berry-type quantities: Application to nonlinear transport, [Xiaoxiong Liu](#), M. Á. Jiménez, S. S. Tsirkin, I. Souza, in progress.
4. 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
5. Origin of spin reorientation and intrinsic anomalous Hall effect in the kagome ferrimagnet TbMn_6Sn_6 , DC Jones, S Das, H Bhandari, [Xiaoxiong Liu](#), P Siegfried, MP Ghimire, SS Tsirkin, II Mazin, NJ Ghimire, arXiv e-prints, arXiv: 2203.17246
6. Triple nodal points characterized by their nodal-line structure in all magnetic space groups, PM Lenggenger, [Xiaoxiong Liu](#), T Neupert, T Bzdušek, arXiv preprint arXiv:2201.08404
7. 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)
8. Unconventional chiral charge order in kagome superconductor KV_3Sb_5 , 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 Lenggenger, [Xiaoxiong Liu](#), T Neupert, T Bzdušek, arXiv preprint arXiv:2104.11254
10. From triple-point materials to multiband nodal links, PM Lenggenger, [Xiaoxiong Liu](#), SS Tsirkin, T Neupert, T Bzdušek, **Physical Review B** 103 (12), L121101, (2021)
11. 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, arXiv preprint arXiv:2101.05763
12. Magneto-transport and Shubnikov–de Haas oscillations in the type-II Weyl semimetal candidate NbIrTe_4 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)
13. Quantum anomalous Hall effect and topological phase transition in two-dimensional antiferromagnetic Chern insulator NiO_2Cl_6 , WW Yang, L Li, JS Zhao, [Xiaoxiong Liu](#), JB Deng, XM Tao, XR Hu, **Journal of Physics: Condensed Matter** 30 (18), 185501, (2018)
14. 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)
15. 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)

16. 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)
17. 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)
18. 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)