



# Xiaoxiong Liu

## Curriculum Vitae

### General

Born 2nd Feb 1993  
Nationality China  
E-mail [xxliu@physik.uzh.ch](mailto: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.  
Thesis: Simulation of Nonlinear Electronic Transport Using Wannier Interpolation. Supervisor: Stepan S. Tsirkin, Group leader: Titus Neupert  
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: Jianbo Deng  
2012–2016 **B.Sc. in Physics**, *Lanzhou University*, China.  
Thesis: First-principle Investigations of 3d Transition Metal (Fe, Cu, and Co)-doped Rock-salt MgO by Chain. Supervisor: 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.

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## Languages

Chinese **Native**  
English **Professional Fluency**

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## 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>

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## 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](https://github.com/Liu-Xiaoxiong/symmetrize_wann_matrix)

### Co-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>

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## 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>

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## Publication Activity

17 Publications, including: Nature Material(1), Communications Physics(1), PRL(2), PRB(4), APL(1)

453 citations.

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## References

- Group Leader **Titus Neupert**, Institut-Physik, University of Zurich, <neupert@physik.uzh.ch>.  
Supervisor **Stepan S. Tsirkin**, Centro de Física de Materiales, Universidad del País Vasco, <stepan.tsirkin@ehu.eus>.  
Collaborator **Ivo Souza**, Centro de Física de Materiales, Universidad del País Vasco <ivo\_souza@ehu.eus>.

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## Participation in Conferences

### Oral Contributions

1. Ab initio calculations of electrical magnetochiral anisotropy with Wannier interpolation, **APS March meeting**, Las Vegas, USA, March 5-10, 2023
2. Symmetrization of berry curvature and magnetic moment, **Wannier 2022 Developers Meeting (smr 3757)**, ICTP, Trieste, Italy, May 23-27, 2022
3. 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. Electrical magnetochiral anisotropy in trigonal tellurium from first principles  
[Xiaoxiong Liu](#), Ivo Souza, Stepan S. Tsirkin, **arXiv e-prints**, arXiv:2303.10164
2. Covariant derivatives of Berry-type quantities: Application to nonlinear transport  
[Xiaoxiong Liu](#), Stepan S. Tsirkin, Ivo Souza, **arXiv e-prints**, arXiv:2303.10129
3. Origin of spin reorientation and intrinsic anomalous Hall effect in the kagome ferrimagnet  $\text{TbMn}_6\text{Sn}_6$   
DC Jones, S Das, H Bhandari, [Xiaoxiong Liu](#), P Siegfried, MP Ghimire, SS Tsirkin, II Mazin, NJ Ghimire, **arXiv e-prints**, arXiv: 2203.17246
4. Emergent Edge Modes in Shifted Quasi-One-Dimensional Charge Density Waves  
SB Zhang, [Xiaoxiong Liu](#), MS Hossain, JX Yin, MZ Hasan, T Neupert, **Physical Review Letters** 130, 106203, (2023)
5. Triple nodal points characterized by their nodal-line structure in all magnetic space groups  
PM Lenggenhager, [Xiaoxiong Liu](#), T Neupert, T Bzdušek, **Physical Review B** 106 (8), 085128, (2022), (共同通信)
6. Universal higher-order bulk-boundary correspondence of triple nodal points  
PM Lenggenhager, [Xiaoxiong Liu](#), T Neupert, T Bzdušek, **Physical Review B** 106 (8), 085129, (2022)
7. Intriguing magnetism of the topological kagome magnet  $\text{TbMn}_6\text{Sn}_6$   
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)
8. 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), (共同一作)
9. Unconventional chiral charge order in kagome superconductor  $\text{KV}_3\text{Sb}_5$   
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)
10. 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)
11. Magneto-transport and Shubnikov-de Haas oscillations in the type-II Weyl semimetal candidate  $\text{NbIrTe}_4$  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), (共同一作)

12. Quantum anomalous Hall effect and topological phase transition in two-dimensional antiferromagnetic Chern insulator  $\text{NiOsCl}_6$   
WW Yang, L Li, JS Zhao, [Xiaoxiong Liu](#), JB Deng, XM Tao, XR Hu, **Journal of Physics: Condensed Matter** 30 (18), 185501, (2018)
13. A nonmagnetic topological Weyl semimetal in quaternary Heusler compound  $\text{CrAlTiV}$   
[Xiaoxiong Liu](#), L Li, Y Cui, J Deng, X Tao, **Applied Physics Letters** 111 (12), 122104, (2017)
14. Ternary Weyl semimetal  $\text{NbIrTe}_4$  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)
15. First-principle investigations of 3d transition metal (Fe, Cu, and Co)-doped rocksalt  $\text{MgO}$  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)
16. Effect of As and Nb doping on the magnetic properties for quaternary Heusler alloy  $\text{FeCoZrGe}$   
GY Mao, [Xiaoxiong Liu](#), Q Gao, L Li, HH Xie, G Lei, JB Deng, **Journal of Magnetism and Magnetic Materials** 398, 1-6, (2016)
17. First-principle study of half-metallic ferromagnetism in rocksalt  $\text{XO}$  ( $\text{X} = \text{Li, K, Rb, Cs}$ )  
G Lei, [Xiaoxiong Liu](#), HH Xie, L Li, Q Gao, JB Deng, **Journal of Magnetism and Magnetic Materials** 397, 176-180, (2016)