Final Report for DOE Award DE-SC0018945

Predictive Theory of Topological States of Matter

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Award Duration: 2018-2021

Abstract

This DOE award supported the PI's research on topological quantum materials between 2018 and 2021. The PI developed predictive theories for new classes of topological insulators and topological/unconventional superconductors and identified their material realizations in collaboration with experimentalists. The PI theorized new topological transport phenomena, including spin superfluidity in moire materials and the superconducting diode effect. Topological transport phenomena have potential applications in cryogenic computing, low-power electronics, high-frequency rectification, infrared detection, energy harvesting and thermoelectric application. By discovering new quantum materials and new functional properties, the PI's research contributed significantly to the advancement of DOE scientific and technological base, especially in energy frontier research.

The PI's research supported by this DOE award studies novel and topological states of matter and their material realization. These include (1) topological insulators with chiral edge states supporting dissipationless charge current; (2) superconducting diodes that exhibit zero resistance in the forward direction and finite resistance in the backward direction; (3) nonceontrosymmetric conductors that exhibit intrinsic nonlinear current-voltage characteristics, which enable high-frequency current rectification without invoking any junction; (4) unconventional superconductors in which mobile electrons attract due to their repulsion with localized electrons.

The award has supported the PI to train students and postdocs in frontier research in theoretical condensed matter physics and engage them in collaboration with leading experimental groups. The efforts of the PI's group over the three-year period have results in 14 publications.

Below is a summary of main achievements of the PI supported by this DOE award.

1. Topological Chern insulators

By performing large-scale density functional theory calculations, the PI's group recently identified topological moire bands with valley-contrasting Chern number in the semiconductor moire heterostructure MoTe2/WSe2 [PNAS 2021]. This work paved the way for understanding the microscopic origin of the quantum anomalous Hall (QAH) effect in this semiconductor heterostructure discovered by Cornell group in collaboration with the PI. The observed QAH state is robust and reproducible, holding great promise for achieving dissipationless transport at higher temperatures in in transition metal dichalcogenide heterostructures. The identification of topological flat bands in semiconductor bilayers also provides a promising venue to search for fractional quantum anomalous Hall effect at zero magnetic field.

2. Topological and finite-momentum superconductors

The PI and his experimental collaborators discovered [Science 2021] a novel superconducting state with finite momentum pairing in proximitized topological insulator film Bi2Te3/NbSe2. The finite Cooper pair momentum arises from Messner effect under a small parallel magnetic field. Remarkably, the Fermi surface of Dirac surface states is partly gapped and partly gapless. The existence of such a segmented Fermi surface in current-carrying superconductors was first predicted by Peter Fulde more than 50 years ago, abut has never been observed directly until this work. This segmented Fermi surface also provides a new route to creating Majorana fermions with very low magnetic fields.

The PI and coworker also established the phase diagram of finite momentum superconductivity in inversion-breaking 2D materials due to the Zeeman effect [PNAS 2021]. They further identified a remarkable supercurrent diode effect as a direct probe of finite momentum pairing [PNAS

2022]. The PI's work is the first microscopic theory of intrinsic superconducting diode effect. This effect has potential applications in superconducting circuits for cryogenic computing.

3. Topological quantum transport

The PI and his student Michal Papaj theorized a new type of nonlinear Hall effect at B=0 in ballistic regime, dubbed "Magnus Hall effect" [PRL 2019]. This effect arises from the Berry curvature of Bloch electrons moving under an built-in electric field, which produces a transverse velocity and hence the Hall effect. The Magnus Hall effect enables current rectification at high frequency and low input power, which opens door to potential applications in THz electronics, RF/THz sensing, and energy harvesting.

The PI and coworker also proposed spin superfluidity due to xy antiferromagnetism in the Mott insulator state in twisted semiconductor bilayers [Nature Communications 2021]. Spin superfluidity enables long-distance spin transport with reduced energy dissipation.

4. Unconventional superconductivity in moire materials

The PI studied unconventional superconductivity in two dimensional materials. With his student Vlad Kozii, the PI proposed nematic superconductivity in twisted bilayer graphene, which is stabilized by spin density wave fluctuations [PRB 2019]. With his student Valentin Crepel, the PI introduced a new mechanism and an exact theory of superconductivity from strong repulsion in multi-band systems, where the pairing interaction arises from high-energy interband excitations [Science Advances 2021, PNAS 2022].

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List of publications supported by this DOE award:

1. N. F. Q. Yuan and L. Fu, "Supercurrent diode effect and finite-momentum superconductors", ***Proceedings of the National Academy of Sciences***, 119, e2119548119 (2022).
2. V. Crépel and L. Fu, "Spin-triplet superconductivity from excitonic effect in doped insulators", ***Proceedings of the National Academy of Sciences*** 119, e2117735119 (2022).
3. R. M. Fernandes and L. Fu, "Charge-4e Superconductivity from Multicomponent Nematic Pairing: Application to Twisted Bilayer Graphene", ***Physical review letters*** 127, 047001 (2021).
4. V. Crépel and L. Fu, "New mechanism and exact theory of superconductivity from strong repulsive interaction", ***Science Advances*** 7, eabh2233 (2021).
5. Y. Zhang, T. Devakul and L. Fu, "Spin-textured Chern bands in AB-stacked transition metal dichalcogenide bilayers", ***Proceedings of the National Academy of Sciences*** 118, e2112673118 (2021).
6. Z. Zhu, M. Papaj, X. Nie, H. Xu, Y. Gu, X. Yang, D. Guan, S. Wang, Y. Li, C. Liu, J. Luo, Z. Xu, H. Zheng, L. Fu and J. Jia, "Discovery of segmented Fermi surface induced by Cooper pair momentum", ***Science*** 374, 1381 (2021).
7. N. Yuan and L. Fu, "Topological metals and finite-momentum superconductors" ***Proceedings of the National Academy of Sciences*** 118, e2019063118 (2021).
8. Z. Bi and L. Fu, "Excitonic density wave and spin-valley superfluid in bilayer transition metal dichalcogenide", ***Nature Communications*** 12, 642 (2021).
9. K. Slagle and L. Fu, "Charge Transfer Excitations, Pair Density Waves, and Superconductivity in Moiré Materials", ***Physical Review B*** 102, 235423 (2020).
10. M. Papaj and L. Fu, "Magnus Hall Effect", ***Phys. Rev. Lett.*** 123, 216802 (2019).
11. N. F. Q. Yuan, H. Isobe and L. Fu, "Magic of high order van Hove singularity", ***Nature Communications*** 10, 5769 (2019).
12. C. H. Hsu, X. Zhou, T. R. Chang, Q. Ma, N. Gedik, A. Bansil, S. Y. Xu, H. Lin and L Fu, "Topology on a new facet of bismuth", ***Proceedings of the National Academy of Sciences*** 116, 13255 (2019).
13. V. Kozii, H. Isobe, J. W. F. Venderbos and L. Fu, "Nematic superconductivity stabilized by density wave fluctuations: Possible application to twisted bilayer graphene", ***Phys. Rev. B*** 99, 144507 (2019).
14. Zhen Bi, Noah F. Q. Yuan, Liang Fu, "Designing Flat Band by Strain", ***Phys. Rev. B*** 100, 035448 (2019).

PhDs granted to students supported:

1. Valentin Crepel (graduated in 2022, postdoc fellow at Flatiron Institute)
2. Michal Papaj (graduated in 2021, Moore postdoc fellow at UC Berkeley)
3. Vlad Kozii (graduated in 2019, Assistant Professor at Carnegie Mellon University)

Graduate students supported:

1. Valentin Crepel
2. Michal Papaj
3. Vlad Kozii
4. Tongtong Liu

Postdocs supported:

1. Noah Yuan
2. Yang Zhang