Final Technical Report of DOE Grant Number: DE-SC0002554
Focused Research Group in Correlated Electron and Complex Materials

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I. OVERVIEW

While the remarkable physical properties of correlated and complex electronic materials hold great promise for technological applications, one of the key values of the research in this field is its profound impact on fundamental physics. The *transition metal oxides*, *pnictides*, and *chalcogenides* play a key role and occupy an especially important place in this field. The basic reason is that the outer shell of transition metals contains the atomic *d*-orbitals that have small spatial extent, but not too small to behave as localized orbtials. These *d*-electrons therefore have a small wave function overlap in a solid, *e.g.* in an octahedral environment, and form energy bands that are relatively narrow and on the scale of the short-range intra-atomic Coulomb repulsion (Hubbard *U*). In this intermediate correlation regime lies the challenge of the many-body physics responsible for new and unconventional physical properties.

The study of correlated electron and complex materials represents both the challenge and the vitality of condensed matter and materials physics and often demands close collaborations among theoretical and experimental groups with complementary techniques. Our team has a track record and a long-term research goal of studying the unusual complexities and emergent behaviors in the charge, spin, and orbital sectors of the transition metal compounds in order to

gain basic knowledge of the quantum electronic states of matter. During the funding period of this grant, the team continued their close collaborations between theory, angle-resolved photoemission spectroscopy, and scanning tunneling microscopy and made significant progress and contributions to the field of iron-based superconductors, copper-oxide high-temperature superconductors, triangular lattice transition metal oxide cobaltates, strontium ruthenates, spin orbital coupled iridates, as well as topological insulators and other topological quantum states of matter. These results include both new discoveries and the resolution to outstanding and unresolved issues. It should be emphasized that the DOE funding provided the crucial support for the close and meaningful collaborations of the focused research group that go far beyond simply putting the research papers from each group together. Indeed, the majority of the publications involved multiple PIs and collaborations between theory and experiments.

II. SUMMARY OF RESULTS

During the grant period, the research activities have led to 40 publications, including 3 in *Nature Physics*, 9 in *Physical Review Letters*, 1 *in Physical Review X*, 3 in *Nature Communications*, and 2 in *Nature Materials*. Most of the 40 publications are coauthored with multiple PIs from the focused research group and involved close collaborations between theory and experiments. These are testimonials to the success of our collaborative efforts supported by this DOE grant that have led to important contributions to the proposed fields that are otherwise difficult if not impossible to achieve.

Development of human resources

The funding has helped providing partial support for 7 graduate students; all of them completed their Ph.D. degrees and received postdoc and research associates offers at other institutions.

Dr. Francis Niestemski (postdoc at Stanford)
Dr. Yuan-ming Lu (now Assistant Professor at Ohio State University)
Dr. Madhab Neupane (now Assistant Professor at University of Central Florida)
Dr. Yiming Xu (now Associate Editor at Physics Review X)
Dr. Liang Niestemski (now Assistant Professor at Western New England University)
Dr. Meng Gao (Research scientist at University of Singapore)
Dr. Jihua Ma (Research scientist at Solectria Renewables)

The funding has provided postdoctoral support.

Dr. Sen Zhou (Associate Professor at Institute for Theoretical Physics, Chinese Academy of Sciences, Beijing, China).
Dr. Kaiyu Yang (Senior Researcher at Brion Technologies)
Dr. Yoshinori Okada (Assistant Professor at Tohoku University in Japan)

Estimate of unexpended funds

There are no unexpended funds left.

Highlights of results:

A. Fe-PNICTIDE SUPERCONDUCTORS

- **Electronic structure and pairing symmetry in iron-based superconductors.**
  Europhysics Letters **83**, 47001 (2008)

  The discoveries have been featured in *EuroPhysics News* of the European Physical Society, *Physics Trends* of the American Physical Society, and the *Science News* of Japan. The paper has received over 600 citations thus far, and has been selected as a "Fast Breaking Paper" by *ScienceWatch*.

- **Zero-energy Majorana-like bound state in iron-based superconductor Fe(Te,Se)**
  Nature Physics, **11**, 543 (2015).

- **Electronic nematicity and the band degeneracy splitting in FeSe**
  Physical Review B **91**, 214503 (2015).

- **Three-dimensional superconducting gap function in optimally-doped iron-pnictides**
  Nature Physics **7**, 198 (2011).

- **Theory of electron correlation and magnetic order in iron-pnictides**
  Physical Review Letters **105**, 096401 (2010).

- **Superconductivity mediated by charge fluctuations in Fe-pnictides**
  Phys. Rev. B **84**, 140505(R) (2011).

- **Effect of uniaxial strain on the structural and magnetic phase transitions**
  Physical Review Letters, **108**, 087001, (2012).

- **Fermi surface dichotomy of superconducting gap and pseudogap in underdoped pnictides**
  Nature Communications **2**, 392 (2011).

B. High-*Tc* cuprate superconductors and physics of Mott inslators

- **Doublon-holon binding, Mott transition, and fractionalized antiferromagnets**
  Physical Review B **89**, 195119 (2014).

- **Valence Bond Glass (VBG) as a unified theory of electronic disorder and the pseudogap phenomena in high temperature superconductors**
  Physical Review Letters **102**, 107001 (2009)

- **Evolution of Fermi surface and normal-state gap in chemically substituted cuprates**
  Physical Review B **79**, 092507 (2009).

- **Electron-Spin Excitation Coupling in an Electron Doped Copper Oxide Superconductor,** Nature physics 7, 719 (2011).

- **Coexistence of competing orders in the high temperature superconductors with two energy gaps in real and momentum space**,
  Physical Review Letters **101**, 207002 (2008)

C. Ruthenates, cobaltates, iridates, and other transition metal oxides

- **Carrier localization and electronic phase separation in bilayer iridates,**
  Nature Communications **5**, 3377 (2014).

- **The evolution of metallic states in a spin-orbit interaction driven correlated iridates**
  Nature Materials, **12** (2013).

- **Spin ordering and electronic texture in the bilayer iridates Sr3Ir2O7**
  Physical Review B **86**, 100401(R) (2012).

- **Observation of a novel orbital selective Mott transition in Ca1.8Sr0.2RuO4**,
  Physical Review Letters **103**, 097001 (2009).

- **Pssible interaction-driven topological phases in (111) bilayers of LaNiO3**
  Physical Review B **84**, 201104 (2011).

- **Nodal *d+id* Pairing and Topological Phases on the Triangular Lattice of $Na_xCoO_2.yH_2O$: Evidence for an Unconventional Superconducting State**
  Physical Review Letters **101**, 217002 (2008).

- **Possible interaction-driven topological phases in (111) bilayers of $LaNiO_3$**
  Phys. Rev. B **84**, 201104(R) (2011).

D. Fractional Quantum Hall Effect, Topological Insulators and other topological states of matter

- **Correlation-hole induced paired quantum Hall states in lowest Landau level**
  Physical Review Letters **105**, 115124 (2010)

- **Quasiparticle interference in magnetically doped topological insulator Bi_2Te_3**
  Physical Review Letters **106**, 206805 (2011)

- **Visualizing Landau Levels of Dirac electrons in a one-dimensional potential**
  Physical Review Letters, **109**, 166407 (2012).

III. List of Publications:

1. J.-X. Yin, Zheng Wu, J.-H. Wang, Z.-Y. Ye, Jing Gong, X. -Y. Hou, Lei Shan, Ang Li, X. -J. Liang, X.-X. Wu, Jian Li, C.-S. Ting, Z. Wang, J.-P. Hu, P.-H. Hor, H. Ding, S. H. Pan, "Observation of a Robust Zero-energy Bound State in Iron-based Superconductor Fe(Te,Se)", **Nature Physics**, vol. 11, 543 (2015).

2. Ilija Zeljkovic, Kane L Scipioni, Daniel Walkup, Yoshinori Okada, Wenwen Zhou, Raman Sankar, Guoqing Chang, Yung Jui Wang, Hsin Lin, Arun Bansil, Fangcheng Chou, Ziqiang Wang, Vidya Madhavan, "Nanoscale Determination of the Mass Enhancement Factor in the Lightly-Doped Bulk Insulator Lead Selenide", **Nature Communications**, vol. 6, 6559 (2015).

3. Y. M. Dai, H. Miao, L. Y. Xing, X. C. Wang, P. S. Wang, H. Xiao, T. Qian, P. Richard, X. G. Qiu, W. Yu, C. Q. Jin, Z. Wang, P. D. Johnson, C. C. Homes, H. Ding, "Spin-Fluctuation-Induced Non-Fermi-Liquid Behavior with suppressed superconductivity in LiFe1-xCoxAs", **Physical Review X**, vol. 5, 031035 (2015).

4. P. Zhang, T. Qian, P. Richard, X. P. Wang, H. Miao, B. Q. Lv, B. B. Fu, T. Wolf, C. Meingast, X. X. Wu, Z. Q. Wang, J. P. Hu, H. Ding, "Observation of two distinct dxz/dyz band splittings in FeSe", **Physical Review B**, vol. 91, 214503 (2015).

5. Junfeng He, T. Hogan, Thomas R. Mion, H. Hafiz, Y. He, J. D. Denlinger, S.-K. Mo, C. Dhital, X. Chen, Qisen Lin, Y. Zhang, M. Hashimoto, H. Pan, D. H. Lu, M. Arita, K. Shimada, R. S. Markiewicz, Z. Wang, K. Kempa, M. J. Naughton, A. Bansil, S. D. Wilson, Rui-Hua He, "Spectroscopic evidence for negative electronic compressibility in a quasi-three-dimensional spin-orbit correlated metal", **Nature Materials**, vol. 14, 577 (2015).

6. Sen Zhou, Yupeng Wang, and Ziqiang Wang, "Doublon-holon binding, Mott transition, and fractionalized antiferromagnet in the Hubbard model". **Physical Review B**, vol. 89, p. 195119 (2014).

7. Chetan Dhital, Tom Hogan, Wenwen Zhou, Xiang Chen, Zhensong Ren, Mani Pokharel, Yoshinori Okada, M. Heine, Wei Tian, Z. Yamani, C. Opeil, J.S. Helton, J.W. Lynn, Ziqiang Wang, Vidya Madhavan & Stephen D. Wilson, "Carrier localization and electronic phase separation in a doped spin-orbit-driven Mott phase in Sr3(Ir1−xRux)2O7". **Nature Communications**, vol. 5, p. 3377 (2014).

8. Yue Yu, Zhuxi Luo, and Ziqiang Wang, "Effects of dipole–dipole interaction between cigar-shaped BECs of cold alkali atoms: towards inverse-squared interactions". **Journal of Physics: Condensed Matter** vol. 26, p. 305402 (2014).

9. H. Miao, L.-M. Wang, P. Richard, S.-F. Wu, J. Ma, T. Qian, L.-Y. Xing, X.-C. Wang, C.-Q. Jin, C.-P. Chou, Z. Wang, W. Ku, and H. Ding, "Coexistence of orbital degeneracy lifting and superconductivity in iron-based superconductors", **Physical Review B**, vol. 89, p. 220503(R) (2014).

10. Chetan Dhital, Tom Hogan, Z. Yamani, Robert J. Birgeneau, W. Tian, M. Matsuda, A. S. Sefat, Ziqiang Wang, and Stephen D. Wilson, "Evolution of antiferromagnetic susceptibility under uniaxial pressure in Ba(Fe1−xCo x)2As2", **Physical Review B**, vol. 89, p. 214404 (2014).

11. L. K. Zeng, X. B. Wang, J. Ma, P. Richard, S. M. Nie, H. M. Weng, N. L. Wang, Z. Wang, T. Qian, and H. Ding, "Observation of anomalous temperature dependence of spectrum on small Fermi surfaces in a BiS2-based superconductor", **Physical Review B**, vol. 90, p. 054512 (2014).

12. Yoshinori Okada, Daniel Walkup, Hsin Lin, Chetan Dhital, Tay-Rong Chang, Sovit Khadka, Wenwen Zhou, Horng-Tay Jeng, Arun Bansil, Ziqiang Wang, Stephen Wilson, Vidya Madhavan, "Imaging the evolution of metallic states in a spin-orbit interaction driven correlated iridate", **Nature Materials**, vol.12, p.707 (2013).

13. Hsin Lin, Tanmoy Das, Yoshinori Okada, M. C. Boyer, W. D. Wise, Michelle Tomasik, Bo Zhen, Eric Hudson, Wenwen Zhou, V. Madhavan, Chung-Yuan Ren, Hiroshi Ikuta, and A. Bansil, "Topological dangling bonds with large spin splitting on the surfaces of Bi_2Se_3", **Nano Letters** 13, 1915 (2013).

14. Chetan Dhital, Sovit Khadka, Z. Yamani, Clarina de la Cruz, T. C. Hogan, S. M. Disseler, Mani Pokharel, K. C. Lukas, Wei Tian, C. P. Opeil, Ziqiang Wang, Stephen D. Wilson, "Spin ordering and electronic texture in the bilayer iridate Sr3Ir2O7", **Physical Review B** vol. 86, p. 100401(R) (2012).

15. Yoshinori Okada, Wenwen Zhou, Chetan. Dhital, D. Walkup, Ying Ran, Z. Wang, Stephen D. Wilson, V. Madhavan, ``Visualizing Landau Levels of Dirac Electrons in a One-Dimensional Potential", **Physical Review Letters**, vol. 109, 166407 (2012).

16. A. Dawn A. Bonnell, D. N. Basov, Matthias Bode, Ulrike Diebold, Sergei V. Kalinin, Vidya Madhavan**,** Miquel Salmeron, Udo D. Schwarz, Paul S. Weiss, "Imaging physical

phenomena with local probes – from electrons to photons, spanning continuum to quantum interactions", **Rev. Mod. Phys.** 84, 1343 (2012).

17. Chetan Dhital, Z. Yamani, Wei Tian, J. Zeretsky, A.S. Sefat, Ziqiang Wang, R.J. Birgeneau, Stephen D. Wilson, "Effect of uniaxial strain on the structural and magnetic phase transitions in $BaFe_2As_2$", **Physical Review Letters**, vol. 108, 087001 (2012).

18. Y.-M. Xu, Y.-B. Huang, X.-Y. Cui, R. Elia, R. Milan, M. Shi, G.-F. Chen, P. Zheng, N.-L. Wang, P.-C. Dai, J.-P. Hu, Ziqiang Wang, H. Ding, "Observation of a ubiquitous three-dimensional superconducting gap function in optimally-doped $Ba_{0.6}K_{0.4}Fe_2As_2$", **Nature Physics**, vol. 7, p. 198 (2011).

19. J. Zhao, F. C. Niestemski, Shankar Kunwar, Shiliang Li, P. Steffens, A. Hiess, H. J. Kang, S. D. Wilson, Z. Wang, P. Dai, V. Madhavan, "Electron-Spin Excitation Coupling in an Electron Doped Copper Oxide Superconductor", **Nature physics**, vol. 7, p. 719 (2011).

20. Y. Okada, C. Dhital, Wen-Wen Zhou, Hsin Lin, S. Basak, A. Bansil, Y. -B. Huang, H. Ding, Z. Wang, S. D. Wilson, V. Madhavan, "Observation of novel interference patterns in $Bi_{2-x}Fe_xTe_{3+\delta}$ by Fourier transform scanning tunneling spectroscopy", **Physical Review Letters**, vol. 106, p. 206805 (2011).

21. S. Zhou, G. Kotliar, and Z. Wang, "Superconductivity driven by charge fluctuations in iron-pnictides", **Phys. Rev. B**, vol. 84, p. 140505(R) (2011).

22. Kai-Yu Yang, Wenguang Zhu, Di Xiao, Satoshi Okamoto, Ziqiang Wang, and Ying Ran, "Possible interaction-driven topological phases in (111) bilayers of $LaNiO_3$", **Phys. Rev. B**, vol. 84, p. 201104(R) (2011).

23. Kai-Yu Yang, Yuan-Ming Lu, and Ying Ran, "Quantum Hall effects in a Weyl semimetal: Possible application in pyrochlore iridates" **Phys. Rev. B**, vol. p. 84, 075129 (2011).

24. X. Liu, Z. Wang, X.C. Xie, and Y. Yu, "Abelian and non-abelian anyons in integer quantum anomalous Hall effect and topological phase transitions via superconducting proximity effect", **Phys. Rev. B,** vol. 83, p. 125105 (2011).

25. M. Neupane, P. Richard, Y.-M. Xu, K. Nakayama, T. Sato, T. Takahashi, A. V. Fedorov, G. Xu, X. Dai, Z. Fang, Z. Wang, G.-F. Chen, N.-L. Wang, H.-H. Wen, H. Ding, "Electron-Hole Asymmetry in Superconductivity of Pnictides Originated from the Observed Rigid Chemical Potential Shift", **Physical Review B**, vol. 83, p. 094522, (2011).

26. H. Ding, K. Nakayama, P. Richard, S. Souma, T. Sato, T. Takahashi, M. Neupane, Y.-M. Xu, Z.-H. Pan, A.V. Federov, Z. Wang, X. Dai, Z. Fang, G.F. Chen, J.L. Luo, and N.L. Wang, "Electronic structure of optimally doped pnictide $Ba_{0.6}K_{0.4}Fe_2As_2$: a comprehensive angle resolved photoemission spectroscopy investigation", **Journal of Physics: Condensed Matter**, vol. 23, p. 135701 (2011).

27. Y.-M. Xu, P. Richard, K. Nakayama, T. Kawahara, Y. Sekiba, T. Qian, M. Neupane, S. Souma, T. Sato, T. Takahashi, H. Luo, H.-H. Wen, G.-F. Chen, N.-L. Wang, Z. Wang, Z. Fang, X. Dai, H. Ding, "Fermi surface dichotomy of superconducting gap and pseudogap in underdoped pnictides", **Nature Communications**, vol. 2, p. 392 (2011).

28. Y.-M. Lu, Y. Ran, P. A. Lee, "Z_2 spin liquid in S=1/2 Heisenberg model on Kagome lattice: A projective symmetry group study of Schwinger-fermion mean-field states", **Phys. Rev. B**, vol. 83, p. 224413 (2011).

29. Y.-M. Lu, Y. Ran, "Z_2 spin liquid and chiral antiferromagnetic phase in Hubbard model on the honeycomb lattice: duality between Schwinger-fermion and Schwinger-boson representations", **Physical Review B**, vol. 84, p. 024420 (2011).

30. Sen Zhou and Ziqiang Wang, "Electron correlation and spin density wave order in iron pnictides", **Physical Review Letters**, vol. 105, p. 096401 (2010).

31. Yuan-Ming Lu, Yue Yu, and Ziqiang Wang, "Correlation-hole induced paired quantum Hall states in lowest Landau level", **Physical Review Letters**, vol. 105, p. 216801 (2010).

32. Yuan-Ming Lu, Xiao-Gang Wen, Zhenghan Wang, Ziqiang Wang, "Non-Abelian Quantum Hall States and their Quasiparticles: from the Pattern of Zeros to Vertex Algebra", **Physical Review B**, vol. 81, p. 115124 (2010).

33. L. R. Niestemski and Ziqiang Wang, "Valence bond glass: A unified theory of electronic disorder and pseudogap phenomena in high temperature superconductors", **Physical Review Letters**, vol. 102, p. 107001 (2009).

34. Chunhua Li and Ziqiang Wang, "Mott and Wigner-Mott transitions in doped correlated electron systems: Effects of superlattice potential and intersite correlation", **Physical Review B**, vol. 80, p. 125130 (2009).

35. M. Neupane, P. Richard, Z.-H. Pan, Y. Xu, R. Jin, D. Mandrus, X. Dai, Z. Fang, Z. Wang, and H. Ding, "Observation of a novel orbital selective Mott transition in $Ca_{1.8}Sr_{0.2}RuO_4$", **Physical Review Letters**, vol.103, p. 097001 (2009).

36. Z.-H. Pan, P. Richard, Y.-M. Xu, M. Neupane, P. Bishay, A. V. Fedorov, H. Luo, L. Fang, H.-H. Wen, Z. Wang, and H. Ding, "`Evolution of Fermi surface and normal-state gap in the chemically substituted cuprates $Bi_2Sr_{2-x}Bi_xCuO_{6+\delta}$", **Physical Review B**, vol. 79, p. 092507 (2009).

37. J.-H. Ma, Z.-H. Pan, F.C. Niestemski, M. Neupane, Y.-M. Xu, P. Richard, K. Nakayama, T. Sato, T. Takahashi, H.-Q. Luo, L. Fang, H.-H. Wen, Ziqiang Wang, H. Ding, V. Madhavan, "Coexistence of competing orders in the high temperature $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ superconductors with two energy gaps in real and momentum space", **Physical Review Letters**, vol. 101, p. 207002 (2008).

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39. H. Ding, P. Richard, K. Nakayama, K. Sugawara,T. Arakane, Y. Sekiba, A. Takayama, S. Souma, T. Sato,T. Takahashi, Z. Wang, X. Dai, Z. Fang, G. F. Chen,J. L. Luo and N. L. Wang, "Observation of Fermi-surface dependent nodeless superconducting gaps in $Ba_{0.6}K_{0.4}Fe_2As_2$", **Europhysics Letters**, vol. 83, p. 47001 (2008).

40. Yue Yu and Ziqiang Wang, "An exactly soluble model with tunable p-wave paired fermion ground states", **Europhysics Letters**, vol. 84 p. 57002 (2008).