石 印 (Yin Shi)

Ph.D. in Materials Science and Engineering

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Education

Ph.D. (2014 - 2020)

The Pennsylvania State University, University Park, USA

- Major: Materials Science and Engineering
- Thesis: "Phase-field study of metal-insulator transition in strongly correlated VO_2" | Advisor: Long-Qing Chen

Main courses: Renormalization Group | Kinetics of Thermodynamics | Thermodynamics of Materials | Crystal Chemistry | Characterization of semiconductors

B.S. (2010 - 2014)

Peking University, Beijing, China

- Major: Physics
- Thesis: "Thermoelectric effect in disordered 2D topological insulators" | Advisor: Ryuichi Shindou

Main courses: Thermodynamics | Statistical Mechanics | Quantum Mechanics | Solid State Physics | Many Body Physics | Non-equilibrium Thermodynamics | Quantum Statistical Mechanics | Theoretical Mechanics | Electrodynamics | Linear Algebra | Group Representation Theory | Methods of Mathematical Physics

Research Experience

Postdoctoral Researcher (10/2020 - 4/2023)

Long-Qing Chen's group, Pennsylvania State University, USA

- Mesoscale simulation of quantum materials
- Dynamical mean-field theory study of magnetotransport in the bilayer Hubbard model

Graduate Research Assistant (8/2014 - 8/2020)

Long-Qing Chen's group, Pennsylvania State University, USA

- Phase-field modeling of the insulator-metal transition in strongly correlated vanadium dioxide
- First-principles calculation of ferroelectrics

Undergraduate Researcher (2013 - 2014)

Ryuichi Shindou's Group, Peking University, China

- Modeling of thermoelectric effect in disordered topological insulators
- Theory of thermoelectric effect induced by electron-phonon interaction

Undergraduate Researcher (2012 - 2014)	**Ji Feng's Group, Peking University, China** › First-principles calculation of topological crystalline insulators › Theory of valley-selective circular dichroism of 2D crystals

Main Research Accomplishments

1. Developed the first coarse-grained model of prototypical strongly correlated material VO_2 and used it to discover various new physics in VO_2 that have potential important applications, including the electric-field-induced abrupt resistive switching, isothermal-charge-injection induced ultrafast insulator-metal transition and domain wall motion, photoexcited transient charge density wave and bias-driven intrinsic electronic phase oscillation and its fundamental frequency limit.
2. Used density functional theory to calculate the surface states of a topological crystalline insulator SnTe and found that proper chemisorption can unfold the topological surface states by passivating trivial dangling bond states and provide an external control of the relative energies of different Dirac nodes, which is particularly desirable in multivalley transport.

Projects

DE-SC0020145 9/2019 - 8/2023

Computational Mesoscale Science and Open Software for Quantum Materials, grant $2750000
U.S. Department of Energy, Office of Science

Ongoing | Participating

NSF DMR-1420620 8/2014 - 8/2019

Multicomponent Assembles for Collective Function, grant $4000000
U.S. National Science Foundation, Materials Research Science and Engineering Centers

Completed | Participated

Skills

Programming	Fortran • c++ • c • Python • Matlab • Mathematica • Comsol • LaTeX
Figure Editing	Adobe Illustrator

Awards

2019	Rober E. Newnham Award for Research Excellence, Department of Materials Science and Engineering, Pennsylvania State University
2012	Second Price in Outstanding Young Scientist Competition, School of Physics, Peking University

Outreach Activities

2018	Arts Fest Kids Day: train high school and college students to show kids simple science experiments
2017	Nanoteacher Workshop: train high school teachers
2017	Exploration U: show kids simple science experiments

Professional Experience

- Journal reviewer for *Nature Communications* and *npj Computational Materials*
- Teaching assistant for undergraduate course MATSE 401: Thermodynamics of Materials
- Proposal writing for DE-SC0020145: Computational Mesoscale Science and Open Software for Quantum Materials

Selected Publications

- **Y. Shi**, V. Gopalan, L.-Q. Chen, "Phase-field model of coupled insulator-metal transitions and oxygen vacancy redox reactions", *Phys. Rev. B* **107**, L201110 (2023).
- **Y. Shi** and L.-Q. Chen, "Sublattice-Dependent Antiferromagnetic Transitions in Rare Earth Nickelates", *Phys. Rev. Lett.* **130**, 186801 (2023).
- L. Jin, **Y. Shi**, F. I. Allen, L.-Q. Chen, J. Wu, "Probing the Critical Nucleus Size in the Metal-Insulator Phase Transition of VO_2", *Phys. Rev. Lett.* **129**, 245701 (2022) (Featured in Physics, Editors' Suggestion).
- **Y. Shi** and L.-Q. Chen, "Intrinsic Insulator-Metal Phase Oscillations", *Phys. Rev. Applied* **17**, 014042 (2022).
- A. Sternbach, F. Ruta, **Y. Shi**, T. Slusar, J. Schalch, G. Duan, A. McLeod, X. Zhang, M. Liu, A. Millis, H.-T. Kim, L.-Q. Chen, R. Averitt, D. N. Basov, "Nanotextured Dynamics of a Light-Induced Phase Transition in VO_2", *Nano Letters* **21**, 9052-9060 (2021).
- **Y. Shi**, A. E. Duwel, D. M. Callahan, Y. Sun, F. Anika Hong, H. Padmanabhan, V. Gopalan, R. Engel-Herbert, S. Ramanathan, L.-Q. Chen, "Dynamics of voltage-driven oscillating insulator-metal transitions", *Phys. Rev. B* **104**, 064308 (2021).
- S. Cheng, M.-H. Lee, R. Tran, **Y. Shi**, X. Li, H. Navarro, C. Adda, Q. Meng, L.-Q. Chen, R. C. Dynes, S. P. Ong, I. K. Schuller, Y. Zhu, "Inherent stochasticity during insulator–metal transition in VO_2", *Proceedings of the National Academy of Sciences* **118**, e2105895118 (2021).
- A. Sood, X. Shen, **Y. Shi**, S Kumar, S.-J. Park, M. Zajac, Y. Sun, L.-Q. Chen, S. Ramanathan, X. Wang, W. C. Chueh, A. M. Lindenberg, "Universal phase dynamics in VO_2 switches revealed by ultrafast operando diffraction", *Science* **373**, 352-355 (2021).
- **Y. Shi** and L.-Q. Chen, "Spinodal electronic phase separation during insulator-metal transitions", *Phys. Rev. B* **102**, 195101 (2020).
- **Y. Shi** and L.-Q. Chen, "Current-Driven Insulator-To-Metal Transition in Strongly Correlated VO_2", *Phys. Rev. Applied* **11**, 014059 (2019).
- D. Lee, B. Chung, **Y. Shi**, K. Song, N. Campbell, F. Xue, G.-Y. Kim, S. Y. Choi, J. P. Podkaminer, T. H. Kim, P. J. Ryan, J.-W. Kim, T. R. Paudel, J.-H. Kang, D. A. Tenne, E. Y. Tsymbal, M. S. Rzchowski, L. Q. Chen, J. Lee, and C. B. Eom, "Isostructural metal-insulator transition", *Science* **362**, 1037–1040 (2018).
- J. M. Munro, H. Akamatsu, H. Padmanabhan, V. S. Liu, **Y. Shi**, L.-Q. Chen, B. K. VanLeeuwen, I. Dabo, and V. Gopalan, "Discovering minimum energy pathways via distortion symmetry groups", *Phys. Rev. B* **98**, 085107 (2018).
- **Y. Shi** and L.-Q. Chen, "Phase-field model of insulator-to-metal transition in VO_2 under an electric field", *Phys. Rev. Materials* **2**, 053803 (2018).
- **Y. Shi**, F. Xue, and L.-Q. Chen,"Ginzburg-Landau theory of metal-insulator transition in VO_2: The electronic degrees of freedom", *Europhys. Lett.* **120**, 46003 (2017).
- **Y. Shi**, M. Wu, F. Zhang, and J. Feng, "(111) surface states of SnTe", *Phys. Rev. B* **90**, 235114 (2014).

References

Dr. Long-Qing Chen

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Dr. Venkatraman Gopalan

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Dr. Aaron Lindenberg

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Declaration

I hereby declare that the information mentioned above is correct up to my knowledge and bear the responsibility for the correctness of the mentioned particulars.

Date : May 24, 2023

Signature (Yin Shi)