

Personal information



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Present address: Institut für Theoretische Physik und Astrophysik,
Universität Würzburg, Germany

Education and Academic Experience

- 2014.10- Humboldt Research Fellow and Visiting lecturer:
“Density Functional Theory and the physics of oxide Heterostructures”, Universität Würzburg, Germany
Host: Prof. Giorgio Sangiovanni and Prof. Ralph Claessen
- 2011-2014 Postdoc in Computational Materials Science ,
Vienna University of Technology, Austria
Advisor: Prof. Karsten Held
- 2005-2011 Ph.D. in Theoretical Solid State Physics,
University of Twente, Enschede, the Netherlands
Supervisor: Prof. Paul J. Kelly
- 2002-2005 Master of Science in Condensed Matter Theory,
Peking University, Beijing, P. R. China
Supervisor: Prof. Zhao-bin Su and Prof. Zhongshui Ma
- 1998-2002 Bachelor of Science in Applied Physics,
Special Class for the Gifted Young, Shanghai Jiaotong University,
Shanghai, P.R. China

Skills

- First-principles density-functional-theory (DFT) calculations
- Tight-binding Hamiltonian, Wannier projection and transport theory
- DFT+dynamical mean field theory (DMFT), strongly correlated and spin-orbit coupled electron systems,

Academic services

- Referee for PRL, PRB, EPL, JPCM, JPD, FWO Postdoctoral Fellow; Supervise two Ph.D students

Research interests: Oxide heterostructures

Transition metal oxides in bulk form exhibit a huge range of physical properties. Heterostructures of transition metal oxides offer the prospect of greatly enhancing these properties or of combining them to realize entirely new properties and functionalities.

To identify novel properties of oxide heterostructures is the goal of our recent theoretical studies. The general scheme of our studies contains four steps: (i) We first perform first-principles density-functional-theory (DFT) calculations of specific materials, (ii) project the DFT results onto maximally localized Wannier orbitals to construct realistic tight-binding (TB) models, (iii) use the TB models as a starting point for follow-up studies such as spin-orbit coupling, DFT+dynamical mean field theory (DMFT), large-scale simulation, or advanced transport, (iv) and finally figure out intrinsic and unique properties of oxide heterostructures and predict experimental observation.

So far, the scheme seems to work quite well; many of our predictions are confirmed by experiments. We have found three important points of oxide heterostructures: electronic and atomic reconstruction [8, 19] tight-binding description of localized d electrons [9, 12], multi-orbital characters [13, 15], polarity induced reconstruction [16, 18].

Publications

- 1. A route to room temperature ferromagnetic ultrathin SrRuO₃ films**
Liang Si, Zhicheng Zhong, Jan M. Tomczak, and Karsten Held
arXiv:1503.00640 Phys. Rev. Lett. under review (2015)
- 2. Tuning Magnetic Curie Temperature in SrRuO₃ Films via SrTiO₃ Capping-layer**
Sean Thomas, Bouwe Kuiper, Jun Hu, Jasper Smit, Zhaoliang Liao, Zhicheng Zhong, Guus Rijnders, Arturas Vailionis, Ruqian Wu, Gertjan Koster, and Jing Xia
Under review (2015)
- 3. Controlled lateral anisotropy in correlated manganite heterostructures by interface-engineered oxygen octahedral coupling**
Z. Liao, M. Huijben, Z. Zhong, N. Gauquelin, S. Macke, R.J. Green, S. van Aert, J. Verbeeck, G. Van Tendeloo, K. Held, G. A. Sawatzky, G. Koster and G. Rijnders
Nat. Mat. under review (2015)
- 4. Unified picture for the colossal thermopower compound FeSb₂**
M. Battiato, J. M. Tomczak, Z. Zhong, and K. Held
Phys. Rev. Lett. accepted (2015)
- 5. Electronics with correlated oxides: SrVO₃/SrTiO₃ as a Mott transistor**
Zhicheng Zhong, Markus Wallerberger, Jan M. Tomczak, Ciro Taranto, Nicolaus Parragh, Alessandro Toschi, Giorgio Sangiovanni, and Karsten Held
arXiv:1312.5989 Phys. Rev. Lett. accepted (2015)
- 6. First Principles Prediction of Topological Phases in Thin Films of Pyrochlore Iridates**
Xiang Hu, Zhicheng Zhong, and Gregory A. Fiete
arXiv:1411.7333 Scientific Reports accepted (2015)
- 7. Giant switchable Rashba effect in oxide heterostructures**
Zhicheng Zhong, Liang Si, Qinfang Zhang, Wei-Guo Yin, Seiji Yunoki, and Karsten Held
Advanced Materials Interfaces 2, 1400445 (2015)

8. **Electronic reconstruction at the isopolar LaTiO₃/LaFeO₃ interface: an X-Ray photoemission and density-functional theory study**
J. E. Kleibeuker, Zhicheng Zhong, H. Nishikawa, A. Muller, F. Pfaff, D. H. A. Blank, M. Sing, G. Koster, K. Held, R. Claessen, and G. Rijnders
Phys. Rev. Lett. 113, 237402 (2014) Cited: 2 times
9. **Anisotropic two-dimensional electron gas at SrTiO₃(110) protected by its native overlayer**
Zhiming Wang, Zhicheng Zhong, Xianfeng Hao, Stefan Gerhold, Bernhard Stoger, Michael Schmid, Jaime Sanchez-Barriga, Andrei Varykhalov, Cesare Franchini, Karsten Held, and Ulrike Diebold
Proc. Natl. Acad. Sci. U.S.A. 111, 3933 (2014) Cited: 11 times
10. **Structural, magnetic, and electrical properties of Li₂Ir_{1-x}Ru_xO₃**
Hechang Lei, Wei-Guo Yin, Zhicheng Zhong, and Hideo Hosono
Phys. Rev. B (Rapid Communications) 89, 020409 (2014) Cited: 4 times
11. **Rocksalt SnS and SnSe: Native topological crystalline insulators**
Yan Sun, Zhicheng Zhong, Tomonori Shirakawa, Cesare Franchini, Dianzhong Li, Yiyi Li, Seiji Yunoki, and Xing-Qiu Chen
Phys. Rev. B 88, 235122 (2013) Cited: 4 times
12. **Quantum confinement in perovskite oxide heterostructures: Tight binding instead of a nearly free electron picture**
Zhicheng Zhong, Qinfang Zhang, and Karsten Held
Phys. Rev. B 88, 125401 (2013) Cited: 7 times
13. **Theory of spin-orbit coupling at LaAlO₃/SrTiO₃ interfaces and SrTiO₃ surfaces**
Zhicheng Zhong, Anna Toth, and Karsten Held
Phys. Rev. B (Rapid Communications) 87, 161102 (2013) Cited: 38 times
14. **Hard x-ray photoemission and density functional theory study of the internal electric field in SrTiO₃/LaAlO₃ oxide heterostructures**
E. Slooten, Zhicheng Zhong, H. Molegraaf, P. Eerkes, S. Jong, F. Masseur, E. Heumen, M. Kruize, S. Wenderich, J. Kleibeuker, M. Gorgoi, H. Hilgenkamp, A. Brinkman, M. Huijben, G. Rijnders, D. Blank, G. Koster, P. J. Kelly, and M. Golden
Phys. Rev. B 87, 085128 (2013) Cited: 16 times
15. **Microscopic understanding of the orbital splitting and its tuning at oxide interfaces**
Zhicheng Zhong, Philipp Wissgott, Karsten Held, and Giorgio Sangiovanni
Euro. Phys. Lett. 99, 37011 (2012) Cited: 7 times
16. **Prediction of thickness limits of ideal polar ultrathin films**
Zhicheng Zhong, G. Koster, and Paul J. Kelly
Phys. Rev. B (Rapid Communications) 85, 121411 (2012) Cited: 8 times
17. **Electrostatic Doping of Graphene through Ultrathin Hexagonal Boron Nitride Films**
Menno Bokdam, Petr A. Khomyakov, Geert Brocks, Zhicheng Zhong, and Paul J. Kelly
Nano Letters 11, 4631 (2011) Cited: 36 times
18. **Polarity-induced oxygen vacancies at LaAlO₃|SrTiO₃ interfaces**
Zhicheng Zhong, P. X. Xu, and Paul J. Kelly
Phys. Rev. B 82, 165127 (2010) Cited: 45 times
19. **Electronic-structure-induced reconstruction and magnetic ordering at the LaAlO₃|SrTiO₃ interface**
Zhicheng Zhong and Paul J. Kelly
Euro. Phys. Lett. 84, 27001 (2008) Best of 2009 Collection Cited: 50 times;

20. **Magnetic Phase Diagram of FeAs based superconductors**
Zhicheng Zhong, Qinfang Zhang, P. X. Xu, Paul J. Kelly
arXiv:0810.3246v1 (2008)
 21. **Enhancement of polarization in a spin-orbit coupling quantum wire with a constriction**
Jun-Feng Liu, Zhicheng Zhong, Lei Chen, Dingping Li, Chao Zhang, and Zhongshui Ma
Phys. Rev. B 76, 195304 (2007) Cited: 21 times
- ResearcherID: B-7675-2009

References

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