

CURRICULUM VITAE of XI DAI

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Personal information

Date of Birth: 21-07-1971
Citizenship: China

PROFESSIONAL PREPARATION

Zhejiang University, China	B.S. Engineering	1993
Zhejiang University, China	M.S. Physics	1996
Institute of Theoretical Physics, CAS, China	Ph.D. Physics	1999

APPOINTMENTS

CAS Distinguished professor	Institute of Physics, CAS	since 2015
Joint professor and Vice Dean	College of Physical Science, UCAS	since 2014
Assistant Director	Institute of Physics, CAS	since 2012
Deputy director	Beijing National laboratory for condensed matter Physics	since 2009
Professor	Institute of Physics, CAS	since 2007
Research assistant professor	Hong Kong University	2004-2007
Postdoc	Rutgers University	2002-2004
Postdoc	Boston College	2001-2002
Postdoc	Hong Kong University of Science and Technology	1999-2001

AWARDS

Young Scientist Prize of Chinese Academy of Sciences	2011.6
Qiushi group prize for science and technology	2011.9
Distinguished Young Scientist Award of National Science Foundation of China	2011.9
The CAS prize for outstanding scientific achievements	2012.1
The OCPA "Achievements in Asia Award"	2012.8
The KC Chou foundation "Fundamental Physics Prize"	2014.5
Listed as "Highly cited researchers" by Thomson Reuters	2014-2016
Outstanding referees by APS journals	2016

CITATIONS

Total citations on web of Science until 2017.4: 15333
Total citations on google scholar until 2017.4: 21273

h-index (based on web of science): 52
h-index (based on google scholar): 57
homepage on Research ID: <http://www.researcherid.com/rid/C-4236-2008>
homepage on Google Scholar: <https://scholar.google.com/citations?user=Rj1ZUIgAAAAJ&hl=en>

SELECTED INVITED TALKS:

2017.2 "Heavy Weyl fermion state in CeRu₄Sn₆", APW-QMS2017, Yongpyong, Korea
2016.12 "The discovery of Weyl semimetals", Chiral matter from Quarks to Dirac semimetals, RIKEN, Tokyo, Japan
2016.10 "Heavy Weyl fermion state in CeRu₄Sn₆", Computational methods towards engineering novel correlated materials, CECAM, Lausanne, Switzerland
2016.10 "Heavy Weyl fermion state in CeRu₄Sn₆", What about U?--Effects of Hubbard interactions and Hund's Coupling in Solids, ICTP, Trieste, Italy
2016.5 "Topological Semimetals with Triply Degenerate Nodal Points in theta-phase Tantalum Nitride", NSF Frontiers of Condensed matter physics: workshop on topological phases of Matter, Wangshington DC, USA
2016.3 "The Weyl semi-metal: a new topological state in condensed matter", 2016 APS march meeting, Baltimore, USA
2016.3 "Dirac and Weyl Fermions in Topological Semimetals", Princeton, USA
2016.1 "International USMM&CMSI Workshop: Frontiers of Materials and Correlated Electron Science", Tokyo, Japan
2015.11 "Searching for topological semi-metals in realistic materials", 2015 MRS Fall meeting, Boston, USA
2015.11 "The Weyl semi-metal: a new topological state in condensed matter", 15th International Conference on Formation of Semiconductor Interfaces, Hiroshima, Japan
2015.10 "LDA+Gutzwiller method and its application to f-electron materials", 2nd International Workshop on Dynamical Mean Field approach for strongly correlated materials, Dresden, Germany
2015.9 "LDA+Gutzwiller method and its application to f-electron materials", The Psi-k Conference on electronic structure and the properties of condensed matter, San Sebastian, Spain
2015.7 "Weyl Semimetal Phase in Transition-Metal Monophosphides", Novel States in Spin-Orbit Coupled Quantum Matter: from Models to Materials, Santa Barbara, CA, USA
2015.6 "Weyl Semimetal Phase in Transition-Metal Monophosphides", Gordon conference on "Topological & Correlated Matter", Hong Kong
2015.6 "Pseudo spin, real spin texture and angle resolved photo emission spectra in SmB₆", Strongly Correlated Topological Insulators: SmB₆ and Beyond, Michigan University, Ann Arbor, USA
2015.5 "LDA+Gutzwiller method and its application to f-electron materials", Electronic Structure Approaches and Applications to Quantum Matter, Santa Fe, New Mexico, USA

2015.1 “Searching for topological semi-metals in realistic materials”, International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, ICTP, Trieste, Italy

2014.3 “Correlated Topological Insulators with Mixed Valence in SmB₆”, 2014 APS march meeting, Denver, USA

2012.2 “Chern Semimetal and the Quantized Anomalous Hall Effect in HgCr₂Se₄”, 2012 APS march meeting, Boston, USA

2010.7 “Searching for realistic Topological Insulators: from Dirac electron to Quantum Anomalous Hall Effect” , ICPS 2010, Seoul, Korea

EXPERTISE

Density Functional Theory & local density approximation;

Dynamic Mean Field Theory;

LDA+Gutzwiller method;

Topological Materials;

Quantum anomalous Hall effect;

Quantum spin Hall effect;

Strongly Correlated Systems;

Rare Earth and Actinides compounds

MAIN ACCOMPLISHMENT

The main accomplishments of Dr. Xi Dai are listed below.

- 1) Using density functional theory, Dr. Dai and his coworkers discovered the most important topological insulators up to now, the Bi₂Se₃ family, which has large and persisting impact in condensed matter physics and material science.
- 2) Dr. Dai proposed with his collaborators that the magnetically doped Bi₂Se₃ family thin film to be a good material platform to realize quantum anomalous Hall effect, the last missing type in the family of quantum Hall effects. The prediction has been proved by the experiments from IOP and Tsinghua University three years later.
- 3) Dr. Dai and his collaborators predicted several important topological semimetals, including the Dirac semimetal Na₃Bi and Weyl semimetal TaAs, which were the first experimentally confirmed topological semimetals in the corresponding categories.
- 4) Dr. Dai developed a new first principle method for strongly correlated materials, the LDA+Gutzwiller method, which now has been widely applied to study the electronic structure of transition metal oxides, rare earth compounds and actinides compounds.
- 5) Dr. Dai and his coworkers developed the dynamical mean field theory for the Actinides compounds and applied it to the electronic structure calculation of delta-Plutonium. Based on that, they predicted the phonon spectrum of the delta-Plutonium, which has been confirmed shortly by inelastic X-ray scattering spectrum.

SELECTED GRANTS

- 1) National 973 program of China (Grant No. 2013CB921700) . “Novel quantum phenomena in solid states”
- 2) Strategic Priority Research Program (B) of the Chinese Academy of Sciences (Grant No. XDB07020100) “Quantum manipulation of exotic states in condensed matter”

- 3) National 973 program of China (No.2011CBA00108), “Unconventional superconductivity in condensed matter”
- 4) National Science foundation of China, Outstanding young researcher award, “Developing new computational methods for correlated and topological states in condensed matter”
- 5) National Science foundation of China, Regular Grant, “Numerical studies on structural phase transitions of Plutonian under pressure”

SELECTED PUBLICATIONS

- 1) Alexey A. Soluyanov, Dominik Gresch, Zhijun Wang, QuanSheng Wu, Matthias Troyer, **Xi Dai** and B. Andrei Bernevig, “A New Type of Weyl Semimetals”, Nature 527, 7579, (2015).
- 2) Rui Yu, Hongming Weng, Zhong Fang, **Xi Dai**, and Xiao Hu, “Topological Node-Line Semimetal and Dirac Semimetal State in Antiperovskite Cu₃PdN”, Phys. Rev. Lett. 115, 036807 (2015)
- 3) Hongming Weng, Chen Fang, Zhong Fang, B. Andrei Bernevig, and **Xi Dai**, “Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides”, Phys. Rev. X 5, 011029 (2015)
- 4) H. Weng, J. Zhao, Z. Wang, Z. Fang and **Xi Dai** , "Topological Crystalline Kondo Insulator in Mixed Valence Ytterbium Borides." Physical Review Letters 112, 016403, (2014)
- 5) H. Weng, **Xi Dai** and Z. Fang, "Transition-Metal Pentatelluride ZrTe₅ and HfTe₅: A Paradigm for Large-Gap Quantum Spin Hall Insulators", Physical Review X 4, 011002, (2014).
- 6) Feng Lu, JianZhou Zhao, Hongming Weng, Zhong Fang, and **Xi Dai**, “Correlated Topological Insulators with Mixed Valence”, Phys. Rev. Lett. 110, 096401 (2013).
- 7) P. N. Ma, S. Pilati, M. Troyer and **X. Dai**, “Density functional theory for atomic Fermi gases”, Nature Physics 8, 601 (2012).
- 8) Z. Wang, Y. Sun, X.-Q. Chen, C. Franchini, G. Xu, H. Weng, **X. Dai** and Z. Fang, “Dirac semimetal and topological phase transitions in A₃Bi (A=Na, K, Rb)”, Physical Review B 85, 195320 (2012).

- 9) Rui Yu, Wei Zhang, Hai-Jun Zhang, Shou-Cheng Zhang, **Xi Dai** and Zhong Fang, "Quantized Anomalous Hall Effect in Magnetic Topological Insulators", *Science* 329, 61, (2010).
- 10) G. Wang, Y. Qian, G. Xu, **X. Dai** and Z. Fang, "Gutzwiller Density Functional Studies of FeAs-Based Superconductors: Structure Optimization and Evidence for a Three-Dimensional Fermi Surface" *Physical Review Letters* 104 , 047002 (2010).
- 11) H. Zhang, C.-X. Liu, X.-L. Qi, **X. Dai**, Z. Fang and S.-C. Zhang, "Topological insulators in Bi₂Se₃, Bi₂Te₃ and Sb₂Te₃ with a single Dirac cone on the surface" , *Nature Physics* 5, 438, (2009).
- 12) Luca de'Medici, S.R. Hassan, Massimo Capone, and **Xi Dai**, "Orbital-Selective Mott transition out of band degeneracy lifting" , *Phys. Rev. Lett.* 102, 126401 (2009).
- 13) X. Deng, L. Wang, **X. Dai**, and Z. Fang, "Local density approximation combined with Gutzwiller method for correlated electron systems: Formalism and applications", *Physical Review B* 79, 075114 (2009).
- 14) **X. Dai**, T. L. Hughes, X. L. Qi, Z. Fang, and S. C. Zhang, "Helical edge and surface states in HgTe quantum wells and bulk insulators", *Physical Review B* 77, 125319 (2008).
- 15) **X. Dai**, S. Y. Savrasov, G. Kotliar, A. Migliori, H. Ledbetter, and E. Abrahams, "Calculated Phonon Spectra of Plutonium at High Temperatures", *Science* 300, 953 (2003).

RESEARCH PLAN

My research interests are mainly concentrated in two fields, the search for exotic topological states in condensed matter systems and the development of the new computational methods for strongly correlated materials. In the first part, I will focus on the search of new topological states in both bulk crystals and 2D materials, i.e. new topological insulators, Dirac semimetals, Weyl semimetals and quantum anomalous Hall systems. In this fast developing research field, the prediction of the right materials is always the key step. In the following three years, the biggest effort of my group will be made to find new Weyl semimetal materials with large separation between Weyl points with opposite chirality and new 2D topological insulators with large band gap, based on which we can design quantum anomalous Hall systems working even at the room temperature. Another

important direction in this field is the topological material design based on the first principle calculations, i.e. the design of new topological state in the interface between two different materials, the quantum well structures or the structure formed by quantum dots and quantum wires. The exotic behavior under magnetic field is a very important issue in the research of topological semimetal. The unique electromagnetic response is one of the key properties of topological semimetals, which leads to chiral anomaly and chiral magnetic effect. However how these systems will behave under strong enough magnetic field, which drives them into quantum limit, is still an open question and will become another focused project for me to study in the coming five years. I believe that I can setup good collaboration with scientists in high magnetic field lab on these interesting problems.

The second part of my research will be devoted to develop more precise and efficient computational methods to study the electronic structure of strongly correlated materials, which is one of the key problems in condensed matter physics. This is a long term research project, which has been carried out in my research group for about ten years, during which we have developed a completely new method, the Gutzwiller density functional theory, and have already applied it to study many interesting correlated materials, i.e. the iron superconductors, Cerium metal and correlated topological insulators. I'm planning to apply the Gutzwiller density functional theory to study some of the interesting correlated materials, i.e. the heavy fermion materials that have the hidden order and the Iridium compounds with exotic magnetic structure. At meanwhile I will develop linear response theory based on the Gutzwiller approximation, which can be applied to calculate the collective modes for the strongly correlated systems. Another research project I am going to pursue in this direction is to develop the dynamical mean field theory to include the spin orbital coupling and crystal field, which is important for the application of LDA+DMFT to 4d/5d transition metal compounds.

There are several types of grants in US suitable for me to apply in future. First of all I can apply for the individual grant of NSF and DOE. Secondly I can apply for the support from the Material Genome project to do material search in rare earth and Actinides compounds. There are few groups in this world, who have the reliable numerical technique to do first principle calculations for rare earth and Actinides compounds, i.e. heavy fermion and Plutonium compounds. The LDA+Gutzwiller method developed in mu group is very suitable for the total energy calculations for these strongly correlated materials. Together with the improved DMFT codes in my group, we will be quite competitive in this field. At last but not least, I can also apply for grants from the private funding agencies. Last year I was invited to join the Princeton team to apply for the support from Simons Foundation. Although we failed last year, we will continue to apply this year and will have bigger chance to succeed this time.

TEACHING EXPERINCE

From last semester, I start to teach “Many particle physics” at the graduate level in University of CAS. This is one of the core courses for the graduate students with physics major in CAS, which mainly covers the Green’s function technique in zero and finite temperature, the interacting electron gas, transport theory for solid systems, Kondo effect, polaron theory and BCS theory of superconductivity. In the coming semester I am going to teach another short course on “topological band theory” in University of CAS, which covers the basic theory for integer quantum Hall effect, topological insulators and topological semimetals.

PHD STIDENTS TRAINED

Name	Graduation Year	Current Affiliation
JiaNing Zhuang	2009	Research Associate in HK Polytechnic University
XiaoYu Deng	2010	Postdoc in Rutgers University, USA
HaiJun Zhang	2010	Professor in Nanjing University Selected by “Junior Thousand talent project”
Lei Wang	2011	Associate Professor in IOP, CAS Selected by “Junior Thousand talent project”
Rui Yu	2011	Associate Professor in Wuhan University Selected by “Junior Thousand talent project”
Li Huang	2011	Associate Professor in 7 th institute of of Chinese Academy of Engineering Physics
Liang Du	2012	Postdoc in UT Austin, USA
HuanHuan Qiu	2012	Assistant professor in JiangXi Normal University
QuanSheng Wu	2013	Postdoc in ETH Zurich, Switzerland
MingFeng Tian	2013	Associate Professor in 9 th institute of of Chinese Academy of Engineering Physics
ZhiJun Wang	2014	Postdoc in Princeton University, USA
Yilin Wang	2016	Postdoc in Brook Haven National Lab, USA

POSTDOC TRAINED

Name	Year	Current Affiliation
Vincent E. Sacksteder	2010-2013	Research Associate in Royal Holloway University of London
Feng Lu	2011-2014	Associate Professor in NanKai University
Haiyan Lu	2015-2017	Assistant Professor in 7 th institute of of Chinese Academy of Engineering Physics

COMMITTEES SERVED

- 1) The international collaboration committee of Institute of Physics, Since 2009
- 2) The postdoc selection committee of Institute of Physics, Since 2009
- 3) The postdoc selection committee of ICAM, 2009-2011
- 4) The academy committee of institute of Physics, Since 2012
- 5) The degree committee of institute of Physics, Since 2012
- 6) The faculty recruitment committee of institute of Physics, Since 2012
- 7) The science committee of “Asia pacific workshop on strongly correlated systems”, Since 2014
- 8) The teaching committee of college of physics, University of CAS, Since 2014
- 9) The management committee of college of physics, University of CAS, Since 2014
- 10) The APS Committee on International Scientific Affairs (CISA), Since 2017

EXPERTS AVAILABLE FOR RECOMMENDATION LETTERS

- 1) Professor Shou-Cheng Zhang, Stanford University, sczhang@stanford.edu
- 2) Professor Fuchun Zhang, Zhejiang University, fuchun@zju.edu.cn & fuchun@hku.hk
- 3) Professor Gabriel Kotliar, Rutgers University, kotliar@physics.rutgers.edu
- 4) Professor Nan Phuan Ong, Princeton University, npo@Princeton.EDU