

# CURRICULUM VITAE

## **Xiuwen Zhang**

Assistant Professor for Research

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### **EDUCATION BACKGROUND**

- **Ph.D. in Condensed Matter Physics**, Institute of Semiconductors, Chinese Academy of Sciences (CAS), Beijing, China 09/2003 ~ 01/2008
- **B.E. in Engineering**, Department of Electronic Engineering, Tsinghua University, Beijing, China 09/1999 ~ 07/2003

### **PROFESSIONAL EXPERIENCES**

- **Assistant Professor for Research**, Office of the Vice Chancellor for Research, University of Colorado at Boulder (UCB), Boulder, CO, USA 04/2014 ~ present
- **Research Assistant Professor**, Department of Physics, Colorado School of Mines (Mines), Golden, CO, USA 01/2011 ~ 03/2014
- **Postdoctoral Researcher**, Chemical and Materials Science Center, National Renewable Energy Laboratory (NREL), Golden, CO, USA 03/2008 ~ 12/2010
- **Project Officer**, School of Electrical and Electronic Engineering, Nanyang Technological University (NTU), Singapore 10/2006 ~ 10/2007

### **SCIENTIFIC PROJECTS**

- “DMREF: Theory-Guided Experimental Search of Designed Topological Insulators and Band-Inverted Insulators”, NSF, USA, 2013-2016.
- “Ternary Copper Nitride Absorbers”, DOE, USA, 2011-2013.
- “Center for Inverse Design”, DOE, USA, 2009-2014.

### **RESEARCH INTERESTS**

- High-throughput prediction of new materials for photovoltaics absorber, topological insulator, transparent conductor, ferroelectrics, piezoelectrics, dielectrics, thermoelectrics, and Li-ion battery applications.
- Genetic Algorithm for simultaneously optimizing material crystal structure and physical properties including dielectric constants, band gap, and elastic constants.
- Charge transportation and Polaronic effects in materials.
- Phonon, defects, and structural stability of semiconducting materials and devices.

- Topological insulators and spintronics.
- Semiconductor nanocrystals, nano lasers, and nano transistors.

### **PROFESSIONAL SKILLS**

- Expertise in software:
  - Ab initio simulation packages: Vienna Ab-initio Simulation Package (VASP), ABINIT Simulation Package, Quantum ESPRESSO, WIEN2k, Materials Studio, Alloy Theoretic Automated Toolkit (ATAT), PLATO for crystal symmetry analysis, Genetic Algorithm based crystal structure searching code.
  - Device simulation packages: Cadence design systems, PROTEL.
  - Programmer: Fortran, Visual Basic, Python, C language, Mathematica, Matlab, Shell, Assembly language.
  - Computer graphics: Xcrysden, Xmgrace, Origin, Vesta.
  - Other Office software: Office, Latex, Scientific Workplace, vi.
- Knowledge of experiment design:
  - Electroplating copper circular patterns as inductance for microelectronic devices.
  - Using surface-mount technology to fabricate radios.
  - Using Cadence design systems to design decoders.
  - Using PROTEL to design printed circuit boards.

### **ACADEMIC AWARDS**

- Extreme Science and Engineering Discovery Environment (XSEDE) Request Allocation Committee (XRAC) Award, USA, 2014.
- Excellent doctoral dissertation nomination award, Chinese Academy of Sciences, China, 2009.
- Dean's Scholarship for excellence of Chinese Academy of Sciences, China, 2007.
- Dean's Scholarship for excellence of Chinese Academy of Sciences, China, 2006.

### **PROFESSIONAL MEMBERSHIPS**

- American Physical Society
- Materials Research Society
- American Chemical Society

### **REFeree OF ACADEMIC JOURNALS**

- Physical Review Letters
- Journal of Materials Chemistry A
- Journal of Materials Chemistry C
- Physical Review B
- Journal of Applied Physics
- Nanotechnology
- RSC Advance
- Physics Letter A

- Physical Chemistry Chemical Physics
- Journal of Physics: Condensed Matter
- Quantum Information & Computation
- Journal of Electronic Materials
- International Journal of Modern Physics B
- Micro & Nano Letters
- Materials Science and Engineering B
- Modern Physics Letters B

#### RECENT PUBLICATIONS

- “Design of TaIrGe: a ternary half-Heusler transparent hole conductor”, F. Yan, X. Zhang, L. Yu, A. Nagaraja, T. O. Mason, and A. Zunger, [arXiv:1406.0872 \(2014\)](#).
- “Hidden spin polarization in inversion-symmetric bulk crystals”, X. Zhang, Q. Liu, J.-W. Luo, A. J. Freeman, and A. Zunger, [Nature Physics 10, 387-393 \(2014\)](#).
- “Mapping the orbital wavefunction of the surface states in three-dimensional topological insulators”, Y. Cao, J. A. Waugh, X.-W. Zhang, J.-W. Luo, Q. Wang, T. J. Reber, S. K. Mo, Z. Xu, A. Yang, J. Schneeloch, G. Gu, M. Brahlek, N. Bansal, S. Oh, A. Zunger, and D. S. Dessau, [Nature Physics 9, 499–504 \(2013\)](#).
- “Theoretical prediction and experimental realization of new stable inorganic materials using inverse design approach”, A. Zakutayev, X. Zhang, A. Nagaraja, L. Yu, S. Lany, T. O. Mason, D. S. Ginley, and A. Zunger, [J. Am. Chem. Soc. 135, 10048–10054 \(2013\)](#).
- “Strong optical absorption in CuTaN<sub>2</sub> nitride delafossite”, M. Yang, A. Zakutayev, J. Vidal, X. Zhang, D. S. Ginley, and F. J. DiSalvo, [Energy & Environmental Science 6, 2994-2999 \(2013\)](#).
- “Crystal structures and metastability of carbon-boron compounds C<sub>3</sub>B and C<sub>5</sub>B”, A. S. Mikhaylushkin, X. Zhang, and A. Zunger, [Phys. Rev. B 87, 094103 \(2013\)](#).
- “Sorting Stable versus Unstable Hypothetical Compounds: The Case of Multi-Functional ABX Half-Heusler Filled Tetrahedral Structures”, X. Zhang, L. Yu, A. Zakutayev, and A. Zunger, [Adv. Funct. Mater. 22, 1425 \(2012\)](#).

#### RECENT PRESENTATIONS

- X. Zhang, “Associating Specific Materials with Topological Insulation Behavior”, [Invited talk](#) at the [American Physical Society 2014 March Meeting](#), Denver, Colorado, USA, March 3-7, 2014.
- X. Zhang, L. Yu, F. Yang, A. Zakutayev, A. R. Nagaraja, T. O. Mason, D. S. Ginley, and A. Zunger, “Discovery of missing multifunctional ABX compounds”,

- Invited talk* at the Materials Research Society 2013 Fall Meeting, Boston, Massachusetts, USA, Dec 1-6, 2013.
- X. Zhang, A. Zakutayev, A. R. Nagaraja, T. O. Mason, D. S. Ginley, and A. Zunger, “Prediction of previously unreported 18-electron ABC materials via first-principles thermodynamics”, *talk* at the American Physical Society 2013 March Meeting, Baltimore, Maryland, USA, Mar 18- 22, 2013.
  - X. Zhang, J. Vidal, J.-W. Luo, and A. Zunger, “False positive and false negative assignment of Topological Insulator in DFT”, *Condensed Matter Seminar* in University of Colorado, Boulder, Colorado, USA, Nov 10, 2011.