

CURRICULUM VITAE

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Education

2009 Ph.D. Michigan State University, East Lansing, Michigan, U.S.A.
Ph.D. Thesis title: ***Electronic and Structural properties of functional nanostructures***
2002 M.S. Nanjing University, Nanjing, Jiangsu, China
1999 B.S. Nanjing University, Nanjing, Jiangsu, China

Professional Experience

2004-2009 Research Assistant at Michigan State University, East Lansing, MI, U.S.A.
2002-2003 Teaching Assistant at Michigan State University, East Lansing, MI, U.S.A.
1999-2002 Research Assistant at Nanjing University, Nanjing, Jiangsu, China

Publications (click on the hyperlinks to access the sources on the web):

(a) In pursuit of my masters degree:

1. T Yang, Z H Wang, H Zhang, Y Nie, J Fang, H Luo, X F Wu and S Y Ding, "In-plane and out-of-plane magnetoresistivity in a MTG Er-doped YBCO crystal" [Superconductor Science and Technology 15, 586-591 \(2002\)](#)
2. T. Yang, Z.H. Wang, H. Zhang, Y. Nie, L. Qiu, "Peak effect in the MTG- $\text{YBa}_{2-x}\text{Na}_x\text{Cu}_3\text{O}_y$ single crystals" [Physica C 386 \(2003\) 69-72](#)
3. T. Yang, Z.H. Wang, H. Zhang, J. Fang, Y. Nie, L. Qiu, S.Y. Ding, "Effective activation energy and phase diagram in the Er-doping MTG- $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ crystal" [Physica C 384 \(2003\) 130-136.](#)

(b) In pursuit of my Ph.D. degree:

4. Teng Yang, Shinya Okano, Savas Berber, and David Tománek, "Interplay between structure and magnetism in $\text{Mo}_{12}\text{S}_9\text{I}_9$ nanowires", [Phys. Rev. Lett. 96, 125502 \(2006\)](#)
5. Igor Popov, Teng Yang, Savas Berber, Gotthard Seifert and David Tománek, "Unique Structural and Transport Properties of Molybdenum chalcogenide nanowires" [Phys. Rev. Lett. 99, 085503 \(2007\)](#)
6. R.K. Raman, Y. Murooka, C.Y. Ruan, T. Yang, S. Berber, D. Tománek, "Direct observation of photo-induced structural changes in graphite" [Phys. Rev. Lett. 101, 077401 \(2008\)](#)
7. Teng Yang, Savas Berber, Jun-Fu Liu, Glen P. Miller, and David Tománek, "Self-assembly of long chain alkanes and their derivatives on graphite" [Journal of Chemical Physics 128, 124709 \(2008\)](#)
8. Teng Yang, Savas Berber and David Tománek, "Compositional ordering and transport properties in $\text{Mo}_6\text{S}_{9-x}\text{I}_x$ nanowires: Ab initio calculations" [Phys. Rev. B 77, 165426 \(2008\)](#)
9. Bogdan Diaconescu, Teng Yang, Savas Berber, Mikael Jazdzzyk, Glen P. Miller, David Tománek, and Karsten Pohl, "Molecular self-assembly of functionalized fullerenes on a metal surface" [Phys. Rev. Lett. 102, 056102 \(2009\)](#)

Oral and poster presentations:

1. **Structural and Electronic Properties of $\text{Mo}_6\text{S}_x\text{I}_{9-x}$ Nanowires.** Contributed talk at the 2005 March Meeting of the American Physical Society in Los Angeles, California, U.S.A. March 24, 2005.
2. **Structural and Electronic Properties of Nanowires.** Contributed PGO seminar talk at Michigan State University, East Lansing, Michigan, U.S.A. March 03, 2006. (Best PGO talk in Spring Semester 2006 and granted Thomas. A. Kaplan award)
3. **Compositional and magnetic ordering in $\text{Mo}_6\text{S}_x\text{I}_{9-x}$ nanowires.** Contributed talk at the 2006 March Meeting of the American Physical Society in Baltimore, Maryland, U.S.A. March 13, 2006.
4. **Interplay between structure and magnetism in $\text{Mo}_6\text{S}_{9-x}\text{I}_x$ nanowires.** Poster presentation at the NT06 conference, Nagano, Japan, June 18 - 23, 2006.
5. **Replicating carbon nanotubes with molybdenum chalcogenide nanowires.** Contributed talk at the 2007 March Meeting of the American Physical Society in Denver, Colorado, U.S.A. March 5 - 9, 2007.
6. **Improving carbon nanotubes with molybdenum chalcogenide nanowires.** Contributed talk at the First symposium on Transition metal chalcogenide nanostructures in Rathen, Germany, March 18 - 21, 2007.
7. **Polymer Ordering on heterogeneous systems.** Contributed talk at the NIRT meeting at Kellogg Biological Station, Hickory Corners, Michigan, U.S.A. August 9 - 11, 2007.

8. **Self-assembly of long chain alkanes and their derivatives on graphite.**

Contributed talk at the 2008 March Meeting of the American Physical Society in New Orleans, Louisiana, March 10 -14, 2008.

9. **Improving carbon nanotubes with molybdenum chalcogenide nanowires.**

Contributed talk of Teng Yang at 2008 PASI (Pan American Advanced Studies Institute) in Buzios, Brazil, March 30 - April 11, 2008

Research Experience

In pursuit of my PhD degree, I have been working on atomic scale electronic and structural properties of nanostructures using *ab initio* Density Functional calculations under the supervision of Professor David Tomanek at Michigan State University. From carbon materials such as graphite and organic polymers to transitional metal chalcogenide nanowires (TMCN), I have been trying to understand both fundamental properties and possible applications.

(1) In one of TMCN or so-called $\text{Mo}_6\text{S}_{9-x}\text{I}_x$ nanowires, I investigated the equilibrium geometry and electronic structure using *ab initio* density functional calculations. The skeleton of these unusually stable nanowires consists of rigid, functionalized Mo octahedra, connected by flexible, bistable sulfur bridges. This structural flexibility translates into a capability to stretch up to ~20% at almost no energy cost. The nanowires change from conductors to narrow-gap magnetic semiconductors in one of their structural isomers.

(2) Using *ab initio* calculations I studied the compositional ordering and quantum transport in $\text{Mo}_6\text{S}_{9-x}\text{I}_x$ nanowires. The skeleton of these nanowires consists of Mo octahedra, which are functionalized by S and I adsorbates and connected by flexible S_3 bridges. The optimum geometries and relative stabilities at different compositions are determined by using density functional theory. I find nanowires with $x=3$ to be particularly stable. Nanowires with other compositions are likely to phase separate into iodine-rich and iodine-depleted domains, some of which should have the $\text{Mo}_6\text{S}_6\text{I}_3$ stoichiometry. Our transport calculations, which are based on the nonequilibrium Green's function formalism, indicate that the nanowires are metallic independent of composition and exhibit a quantum conductance of $G=3G_0$, with the three conductance channels involving the S_3 bridges.

(3) I combined *ab initio* density functional and quantum transport calculations based on the nonequilibrium Green's function formalism to compare structural, electronic, and transport properties of $\text{Mo}_6\text{S}_{6-x}\text{I}_x$ nanowires with carbon nanotubes. I find systems with $x=2$ to be particularly stable and rigid, with their electronic structure and conductance close to that of metallic (13,13) single-wall carbon nanotubes. $\text{Mo}_6\text{S}_{6-x}\text{I}_x$ nanowires are conductive irrespective of their structure, more easily separable than carbon nanotubes, and capable of forming ideal contacts to Au leads through thio groups.

(4) In collaboration with professor Chuan-Yu Ruan and his experimental group who uses ultra-fast electron diffraction with aid of femto-second laser pulse, we found and tried to understand some novel lattice contraction between graphite inter-layers following the photo-excitation.

(5) Combining scanning tunneling microscopy STM measurements with *ab initio* calculations, I studied the self-assembly of long chain alkanes and related alcohol and carboxylic acid molecules on graphite. For each system, we identify the optimum adsorption geometry and explain the energetic origin of the domain formation observed in the STM images. Our results for the hierarchy of adsorbate-adsorbate and adsorbate-substrate interactions provide a quantitative basis to understand the ordering of long chain alkanes in self-assembled monolayers and ways to modify it using alcohol and acid functional groups.

(6) In study of the self-assembly of C_{60} molecules functionalized with long alkane chains on the (111) surface of silver, I find that the conformation of the functionalized C_{60} molecule changes upon adsorption on Ag(111) and that the unit cell size in the self-assembled monolayer is determined by the interactions between the functional groups. C_{60} molecules can be assembled in ordered two-dimensional arrays with intermolecular distances much larger than those in compact C_{60} layers, which is confirmed by scanning tunneling microscopy STM measurements and therefore we propose a novel way to control the surface pattern by appropriate chemical functionalization.

Expertise

Proficiency in FORTRAN language and programming, some experience in HTML and python programming language and matplotlib. Skillful in the software GNUplot, XCrysDen, Molekel, Rasmol/Raswin, Microsoft Office, Microsoft Origin, and operation systems OS Linux, Windows XP.

Expertise in following commercial/noncommercial FORTRAN codes:

SIESTA (*ab initio* electronic structure simulation software using localized basis set);

Quantum-Espresso (*ab initio* electronic structure simulation software using plane-wave basis set);

Atomistix (First-principle simulation software for nanoscale quantum transport properties)

CTPMD (Carbon-Tersoff-Potential-Molecular-Dynamics program)

Honors and prizes (since 2001)

2001	English Contest Champion	(Nanjing, China)
2002	Physics student fellowship	(East Lansing, U.S.A.)
2006	Thomas. A. Kaplan award	(East Lansing, U.S.A.)
2006	Nanotube conference 06 student fellowship	(East Lansing, U.S.A.)
2008	Dissertation Completion Fellowship award	(East Lansing, U.S.A.)