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EDUCATION

- May 2010 Ph.D, Physics, **Tulane University**.
  - Thesis Advisor: John P. Perdew.
  - Thesis title: Revisiting and revising rungs of Jacob's ladder of density functional theory, with application to problems of molecular adsorption on metal surfaces.
- May 2007 M.S, Mechanical Engineering, **Tulane University**.
- May 2004 M.Eng, Mechanical Engineering, **University of Science and Technology of China**.
- May 2001 B.S., Mechanical Engineering, **University of Science and Technology of China**.

PROFESSIONAL APPOINTMENTS

- July 2015 - present Research Associate Professor, Department of Physics, **Temple University**.
- July 2013 - June 2015 Research Assistant Professor, Department of Physics, **Temple University**.
- May 2010 - July 2013 Postdoctoral fellow (Supervisor: John P. Perdew), department of Physics, **Tulane University**.

PROFESSIONAL ACTIVITIES

- **Reviewer,** Physical Review Letters, Physical Review B, Europhysics Letters, Foundations of Physics, Accounts of Chemical Research, Journal of Chemical Theory and Computation, Chemical Physics Letters, Journal of Chemical Physics, Journal of Physical Chemistry, International Journal of Quantum Chemistry, Journal of Physics and Chemistry of Solids, and Surface Science.
- **Reviewer for funding agencies,** Department of Energy (3 proposals).
- **Member,** American Physical Society (APS).
- **Session chair,** M1 of the 2014 APS March meeting on"Recent Advances in Density Functional Theory".

FUNDED GRANT

- One of about 18 senior investigators of a DoE Energy Frontier Research Center: Center for the Computational Design of Functional Layered Materials (Aug. 1, 2014 - July 31, 2018). The total budget is $12 million, and my part of it is $485,243

RESEARCH INTERESTS

- Electronic Structure Theory, Quantum Chemistry, Condensed Matter Physics, Materials Science, and Surface Science.
- Density functional theory (DFT) and time-dependent DFT : Meta generalized gradient approximation and its hybrid, self-interaction correction, van der Waals (vdW) interaction, charge transfer, strong correlation, d- and f-electron systems, band gap.
- Structural and dynamical properties of molecules, liquids, and solids.
- Fundamental properties of two-dimensional (2D) materials and 3D layered materials with and without defects: Optical, electronic, magnetic, thermal, mechanical, and dielectric properties.
- Catalysis: Water splitting, surface adsorption and diffusion, and nanoparticles.
- Energy conversion and storage: Layered-materials-based solar cells, and Li-ion and Li-air batteries.
- Weak interactions in biological systems and soft condensed matter: Cation- and anion-π interactions, hydrogen bonds, and vdW interactions; molecular crystals.

TEACHING EXPERIENCE

- 2013-present Department of Physics, Temple University
  - SP2014, Preliminary Exam Preparation (graduate)
  - FA2013, Elementary classical physics I (undergraduate), Recitation
  - Co-advised and mentored 2 postdoctoral researchers and 3 Ph.D students
- 2007-2013 Department of Physics, Tulane University
  - More than 10 substitute lectures for 'Solid State Physics', 'Quantum Mechanics', and 'Atomic, Molecular Physics'
  - Guest lecturer: Introductory Physics I
  - Teaching Assistant: Physics Lab of Introductory Physics I.
  - 2008 Outstanding Teaching Assistant of the Year from American Association of Physics Teachers.
  - Co-advised and mentored 2 Ph.D students

PUBLICATIONS (Google Scholar citation: 782, h-index: 13 at Dec/2015)

41. Jianwei Sun and Mark R. Pederson, Cheap and Reliable Screening for Minima of Reaction Space: a Manganese Oxide Cluster Decorated with Water, *In preparation.*
40. Haowei Peng, Zenghui Yang, John P. Perdew, and Jianwei Sun, SCAN+rVV10: A Versatile Density Functional, *under review in* **Phys. Rev. Lett.**.
39. Daniil A. Kitchaev, Haowei Peng, Yun Liu, Jianwei Sun, John P. Perdew, and Gerbrand Ceder, The Energetics of MnO_2 Polymorphs in Density Functional Theory, *under review in* **Phys. Rev. Lett.**.
38. Jianwei Sun, Richard C. Remsing, Yubo Zhang, Zhaoru Sun, Adrienn Ruzsinszky, Haowei Peng, Zenghui Yang, Arpita Paul, Umesh Waghmare, Xifan Wu, Michael L. Klein, and John P. Perdew, Accurate First-Principles Structures and Energies of Diversely-Bonded Systems from an Efficient Density Functional, *under review in* **Nat. Chem.**
37. John P. Perdew, Jianwei Sun, Richard M. Martin, and Bernard Delley, Perspectives on Semilocal Density Functionals and Constraint Satisfaction, *under review in* **Int. J. Quant. Chem.**

36. John P. Perdew, Jianwei Sun, Alejandro J. Garza, and Gustavo E. Scuseria, Intensive Atomization Energy: Re-Thinking a Metric for Electronic-Structure-Theory Methods, *under review in* **Zeitschrift fur Physikalische Chemie**
35. Alejandro J. Garza, Ireneusz W. Bulik, Ana G. Sousa Alencar, Jianwei Sun, John P. Perdew, and Gustavo E. Scuseria, Combinations of Coupled Cluster, Density Functionals, and the Random Phase Approximation for Describing Static and Dynamic Correlation, and Van Der Waals Interactions, *accepted by* **Mol. Phys.**
34. Alejandro J. Garza, Gustavo E. Scuseria, Adrienn Ruzsinszky, Jianwei Sun, and John P. Perdew, The Two Pillars: Density and Spin-Density Functional Theories, *accepted by* **Mol. Phys.**
33. Hao Dong, Wei Li, Jianwei Sun, Shuhua Li, and Michael L. Klein, Understanding the Boron Nitrogen Interaction and Its Possible Implications in Drug Design, **J. Phys. Chem. B 119**, 14393 (2015).
32. Akila C. Thenuwara, Samantha L. Shumlus, Nuwan H. Attanayake, Elizabeth Cerkez, Ian G.McKendry, Laszlo Frazer, Eric Borguet, Qing Kang, Michael Zdilla, Jianwei Sun, and Daniel R Strongin, Copper-Intercalated Birnessite as a Water Oxidation Catalyst, **Langmuir 31**, 12807 (2015) **Journal Cover**.
31. Songsong Zhou, Jian Han, Shuyang Dai, Jianwei Sun, and David J. Srolovitz, Van Der Waals Bilayer Energetics: Generalized Stacking-Fault Energy of Graphene, Boron Nitride, and Graphene/Boron Nitride Bilayers, **Phys. Rev. B 92**, 155438 (2015).
30. John P. Perdew, Jianwei Sun, Adrienn Ruzsinszky, Pál D. Mezei, and Gábor I. Csonka, Why Density Functionals Should Not Be Judged Primarily by Atomization Energies, **Periodica Polytechnica Chemical Engineering**, Online First (2015) p8356 (DOI: 10.3311/PPch.8356)
29. Jianwei Sun, Adrienn Ruzsinszky, and John P. Perdew, Strongly Constrained and Appropriately Normed Semilocal Density Functional, **Phys. Rev. Lett. 115**, 036402 (2015).
28. Jianwei Sun, John P. Perdew, and Adrienn Ruzsinszky, Semilocal Density Functional Obeying a Strongly-Tightened Bound for Exchange, **Proc. Natl. Acad. Sci. 112**, 685 (2015).
27. Pál D. Mezei, Gábor I. Csonka, Adrienn Ruzsinszky, and Jianwei Sun, Accurate, Precise, and Efficient Theoretical Methods to Calculate Anion-π Interaction Energies in Model Structures, **J. Chem. Theo. Comp. 11**, 360 (2014).
26. Zhenyu Wang, Jianwei Sun, Yonghong Chen, and Chunming Niu, Adsorption and Deposition of Li2O2 on TiC(111) Surface by First-Principles Calculations, **J. Phys. Chem. Lett. 5**, 3919 (2014).
25. Bing Xiao, Jianwei Sun, Adrienn Ruzsinszky, and John P. Perdew, Testing the Jacobs Ladder of Density Functionals for Electronic Structure and Magnetism of Rutile VO2, **Phys. Rev. B 90**, 085134 (2014).
24. John P. Perdew, Adrienn Ruzsinszky, Jianwei Sun, and Kieron Burke, Gedanken Densities and Exact Constraints in Density Functional Theory, **J. Chem. Phys. 140**, 18A533 (2014).
23. Bing Xiao, Jianwei Sun, Adrienn Ruzsinszky, Jing Feng, Robin Haunschild, Gustavo E. Scuseria, and John P. Perdew,Testing Density Functionals for Structural Phase Transitions of Solids Under Pressure: Si, SiO2 and Zr, **Phys. Rev. B 88**, 184103 (2013).
22. Jianwei Sun, Bing Xiao, Yuan Fang, Robin Haunschild, Pan Hao, Adrienn Ruzsinszky, Gábor I. Csonka, Gustavo E. Scuseria, and John P. Perdew, Density Functionals that Recognize Covalent, Metallic, and Weak Bonds, **Phys. Rev. Lett. 111**, 106401 (2013).
21. Yuan Fang, Bing Xiao, Jianmin Tao, Jianwei Sun, and John P. Perdew, Ice Phases Under Ambient and High Pressure: Insights from Density Functional Theory, **Phys. Rev. B 87**, 214101 (2013).
20. Jianwei Sun, Robin Haunschild, Bing Xiao, Ireneusz W. Bulik, Gustavo E. Scuseria, and John P. Perdew, Semi-Local and Hybrid Meta-Generalized Gradient Approximations Based on the Understanding of the Kinetic-Energy-Density Dependence, **J. Chem. Phys. 138**, 044113 (2013).
19. Pan Hao, Jianwei Sun, Bing Xiao, Adrienn Ruzsinszky, Gábor I. Csonka, Jianmin Tao, Stephen Glindmeyer, and John P. Perdew, Performance of Meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions, **J. Chem. Theo. Comp. 9**, 355 (2013).

18. John P Perdew, Adrienn Ruzsinszky, Jianwei Sun, Stephen Glindmeyer, and Gábor I. Csonka, van der Waals Interaction as a Summable Asymptotic Series, **Phys. Rev. A 86**, 062714 (2012).
17. Bing Xiao, Jianwei Sun, Adrienn Ruzsinszky, Jing Feng, and John P. Perdew, Structural Phase Transitions in Si and SiO2 Crystals via the Random Phase Approximation, **Phys. Rev. B 86**, 094109 (2012).
16. Jianwei Sun, Bing Xiao, and Adrienn Ruzsinszky, Communication: Effect of the Orbital-Overlap Dependence in the Meta Generalized Gradient Approximation, **J. Chem. Phys. 137**, 051101 (2012).
15. Adrienn Ruzsinszky, Jianwei Sun, Bing Xiao, and Gábor I. Csonka, A Meta-GGA Made Free of the Order-of-Limits Anomaly, **J. Chem. Theo. Comp. 8**, 2078 (2012).
14. Pan Hao, Yuan Fang, Jianwei Sun, Gábor I. Csonka, Pier H.T. Philipsen, and John P. Perdew, Lattice Constants from Semilocal Density Functionals with Zero-Point Phonon Correction, **Phys. Rev. B (Editor's suggestion) 85**,014111 (2012).
13. Jianwei Sun, Martijn Marsman, Gábor I. Csonka, Adrienn Ruzsinszky, Pan Hao, Yoon-Suk Kim, Georg Kresse, and John P. Perdew, Selfconsistent Meta-Generalized Gradient Approximation within the Projector-Augmented-Wave Method, **Phys. Rev. B (Editor's suggestion) 84**,035117 (2011).
12. John P Perdew, Adrienn Ruzsinszky, Gabor I Csonka, Lucian A Constantin, and Jianwei Sun, Erratum: Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry, **Phys. Rev. Lett. 106**, 179902 (2011).
11. Jianwei Sun, Martijn Marsman, Adrienn Ruzsinszky, Georg Kresse, and John P. Perdew, Improved Lattice Constants, Surface Energies, and CO Desorption Energies from a Semilocal Density Functional, **Phys. Rev. B (Rapid Communication) 83**,121410 (2011).
10. Jianwei Sun, John P. Perdew and Michael Seidl, Correlation Energy of the Uniform Electron Gas, from an Interpolation between High- and Low-Density Limits, **Phys. Rev. B 81**, 085123 (2010).
9. John P Perdew, Adrienn Ruzsinszky, Gabor I Csonka, Lucian A Constantin, and Jianwei Sun, Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry, **Phys. Rev. Lett. 103**, 026403(2009).
8. John P. Perdew, Adrienn Ruzsinszky, Lucian A. Constantin, Jianwei Sun, and Gbor I. Csonka, Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed, **J. Chem. Theo. Comp. 5**, 902 (2009).
7. Jianwei Sun, Extension to Negative Values of the Coupling Constant of Adiabatic Connection for Interaction-Strength, **J. Chem. Theo. Comp. 5**, 708 (2009).
6. Jianwei Sun and Lucy T. Zhang, Temperature Control Algorithms in DCV-GCMD Simulations of Hydrogen Diffusion in Palladium, **J. Chem. Phys. 127**, 164721 (2007).
5. Jianwei Sun, Minghou Liu, Genxuan Zhang, Xianfeng Zhang, and Yiliang Chen, Effects of the Slip Boundary Condition on the 2D Numerical Simulation of Micronozzles, **Journal of Astronautics (Chinese)** Vol. 26 No. 6, P. 707-711 (2005).
4. Minghou Liu, Jianwei Sun, Zhiliang Li and Yiliang Chen, Numerical Study on Micronozzles, **Journal of Engineering Thermophysics (Chinese)** vol. 26 No. z1 p. 199-202 (2005).
3. Jianwei Sun, Minghou Liu, Genxuan Zhang, Yiliang Chen and Xiaodan Cai, Numerical Simulation on Micro Thruster Sub-Sonic Flow Field, **Journal of University of Science and Technology of China (Chinese)**, Vol. 35, No. 4, p. 563-569 (2005).
2. Minghou Liu, Jianwei Sun, Yiliang Chen and Xiaodan Cai, The Thrust Measurement for Micro Thrusters, **Mechanics in Engineering (Chinese)** Vol. 25, No.3, p.9-14 (2003).
1. Zhuojin Zhu, Xifeng Zhu and Jianwei Sun, Numerical Analysis of Heat Transfer in a Photovoltaic Panel, I: Indoor Cases, **Int. Comm. Heat Mass Transfer.** Vol.29, 497 (2002).

Invited Talks

10. Jianwei Sun, Strongly Constrained and Appropriately Normed (SCAN) Semilocal Density Functional: Accurate and Efficient for Molecules, Liquids, and Solids, **March Meeting of American Physical Society**, Baltimore, Maryland, March 2016.
9. Jianwei Sun, Accurate Structures and Energies from the SCAN MetaGGA, **ICMS-Temple University International Workshop**, the Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, December 2015.
8. Jianwei Sun, Accurate Structures and Energies from the SCAN MetaGGA, **IISER-Temple University International Workshop**, Pune, India, December 2015.
7. Jianwei Sun, Testing and Applications of the SCAN MetaGGA, an Accurate and Efficient Nonempirical Density Functional, **2015 Energy Frontier Research Center (EFRC) PI meeting**, Washington, DC, October 2015.
6. Jianwei Sun, Meta-Generalized Gradient Approximations and MGGA-based Nonlocal Functionals of Density Functional Theory, **The 55th Sanibel Symposium**, St. Simons Island, GA, February 2015.
5. Jianwei Sun, Meta-Generalized Gradient Approximations of Density Functional Theory, **The Nha Trang Workshop 2014—Current Topics in Theoretical Chemistry**, Nha Trang, Vietnam, August 2014.
4. Jianwei Sun, Meta-Generalized Gradient Approximations That Recognize Covalent, Metallic, and Weak Bonds, **The Como Moments summer school**, Como, Italy, August 2013.
3. Jianwei Sun, Meta-Generalized Gradient Approximations of Density Functional Theory and Its Applications, **The City University of Hong Kong**, Hong Kong, February 2013.
2. Jianwei Sun, Meta-Generalized Gradient Approximations of Density Functional Theory and Its Applications, **Xi'an Jiao Tong University**, Xi'an, China, December 2012.
1. Jianwei Sun, Revisiting and Revising Rungs of Jacob's Ladder of Density Functional Theory, with Application to Problems of Molecular Adsorption on Metal Surfaces, **Sandia National Laboratories**, Albuquerque, New Mexico, July 2010.

Contributed Talks

13. Jianwei Sun, John P. Perdew, and Adrienn Ruzsinszky; Strongly Constrained and Appropriately Normed (SCAN) Meta-Generalized Gradient Approximation for Exchange and Correlation, **March Meeting of American Physical Society**, San Antonio, Texas, 2015.
12. Jianwei Sun, Xiaoxing Xi, John P. Perdew, Maria Iavarone, Xifan Wu, and Adrienn Ruzsinszky; Center for the Computational Design of Functional Layered Materials: A New Energy Frontier Research Center at Temple University, **Mid-Atlantic Section Meeting of American Physical Society**, Penn State University, University Park, Pennsylvania, October 2014.
11. Jianwei Sun, John P. Perdew, and Adrienn Ruzsinszky; First beyond-LSDA Density Functional Satisfying a Tight Lower Bound for Exchange, **March Meeting of American Physical Society**, Denver, Colorado, 2014.
10. Jianwei Sun, Bing Xiao, Adrienn Ruzsinszky, and John Perdew; Chemi- and Physisorption Together from a Semilocal Density Functional: Graphene on Ni (111), **March Meeting of American Physical Society**, Baltimore, Maryland, March 2013.
9. Jianwei Sun, John Perdew, Bing Xiao, and Adrienn Ruzsinszky; Effect of the Orbital-overlap Dependence on Meta Generalized Gradient Approximation, **March Meeting of American Physical Society**, Boston, Massachusetts, 2012.

8. Jianwei Sun, Martijn Marsman, Georg Kresse, and John P. Perdew; Self-consistent Meta-GGA for Solids, with Application to the CO Adsorption Puzzle, **March Meeting of American Physical Society**, Portland, Oregon, 2010.
7. Jianwei Sun, and John P. Perdew; Optimal Non-Selfconsistent DFT Calculations: GGA and Meta-GGA Adsorption Energies of CO on Pt(111) Surface, **From Basic Concepts to Real Materials Conference**, Santa Barbara, CA, 2009.
6. Jianwei Sun, Adrienn Ruzsinszky, and John P. Perdew; Density Functional Study of CO Adsorption on d-metal Surface using TPSS Functional; **March Meeting of American Physical Society**, Pittsburgh, PA, 2009.
5. Jianwei Sun, Chen Li and John P. Perdew; Density Functional Study of Hydrogen Adsorption on the (1 1 1) Palladium Surface Using Generalized Gradient Approximation (GGA) Designed for Solids(PBEsol); **Thirteenth International Workshop on Quantum Systems in Chemistry and Physics**, Lansing, MI, July 6-12, 2008.
4. Jianwei Sun, Chen Li and John P. Perdew; Density Functional Study of Hydrogen Adsorption on the (1 1 1) Palladium Surface Using Generalized Gradient Approximation (GGA) Designed for Solids(PBEsol); **School of Science and Engineering Research Day of Tulane University**, New Orleans, LA, 2008.
3. Jianwei Sun, Michael Seidl and John P. Perdew; Correlation Energy of 3D Spin-Polarized Electron Gas: A Single Interpolation between High- and Low-Density Limits; **March Meeting of American Physical Society**, New Orleans, LA, 2008.
2. Jianwei Sun, Dual-Control Volume Grand Canonical Molecular Dynamics (DCV-GCMD) Simulation of Hydrogen Diffusion in Palladium -How can it be related to DFT? **School of Science and Engineering Research Day of Tulane University**, New Orleans, LA, 2007.
1. Jianwei Sun and Lucy Zhang; (DCV-GCMD) Study on Gradient Driven Diffusion of Hydrogen in Palladium; **7th World Congress on Computational Mechanics**, Los Angeles, CA, 2006

REFERENCES

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RESEARCH STATEMENT

Jianwei Sun (jianweisun@temple.edu)

Executive Summary

Due to its efficiency and useful accuracy, density functional theory (DFT), along with its extensions (e.g., the time-dependent or TD DFT), is one of the most widely used electronic structure theories in condensed matter physics and quantum chemistry. DFT is exact for the ground state energy and electron density in principle, but its exchange-correlation energy (E_{xc}) needs to be approximated in practice. My research interests are to understand fundamental properties of E_{xc} (or the exchange-correlation potential V_{xc} and kernel f_{xc} in case of TDDFT), to use such understanding to derive accurate and/or efficient approximations, and to apply the derived approximations to predict properties and behaviors of materials as well as to computationally design materials that are scientifically, technologically, or economically important.

In the past several years, I was focusing on the development of semilocal meta-generalized gradient approximation (meta-GGA) to E_{xc}. I have demonstrated that meta-GGA is more accurate than the current dominant semilocal approximations with comparable computational cost [1]. I have designed a way to construct metaGGAs [2]. I have shown that metaGGAs can recognize different chemical bonds (covalent, metallic, and even weak bonds) and treat them accordingly with different GGAs [3]. I have constructed the strongly-constrained and appropriately-normed (SCAN) metaGGA [4] that predicts accurate structures and energies with improved band gaps for materials and provides the description of the intermediate-range van der Waals (vdW) interaction. By adding the long-range vdW correction, SCAN+ vdW-correction emerges as a promising functional [5] for molecules, layered solids, and non-layered solids, where vdW may or may not be important. I have applied SCAN to study the intercalation of copper in the birnessite manganese oxide for water splitting. Besides the work on metaGGAs, I have found a cheap and reliable way to screen for minima of the reaction space of water oxidation with manganese oxide clusters [6], which can be extended to study mechanisms of chemical reactions and to screen for new catalysts.

Next, with the understanding from SCAN, I will develop nonlocal corrections to SCAN for strongly-correlated electron systems and a metaGGA for accurate band gaps. In the application side at the near future, I will use SCAN and SCAN-based nonlocal functionals (including SCAN+vdW-correction) to study systems and properties important to the energy and health issues. I will keep working on applying the cheap and reliable way to study catalytic problems and to screen for new catalysts.

Background and Challenges of Density Functional Theory

Modern society has been benefitting from developments of technology (e.g., cars, cell phones, computers, etc), which however demand enormous resources from our planet, the Earth, and change our environment dramatically (e.g., climate change). To advance technologies that are environmentally friendly, one of the keys is to develop and control the underlying materials. The real-world materials are collections of atoms, which in turn consist of nuclei surrounded by much lighter electrons. The behavior of electrons is governed by quantum mechanics and largely determines properties of materials. Therefore, the grand challenge becomes how to understand and control materials processes at the level of electrons.

DFT is one of the most widely used approaches to calculate electronic structures of materials due to its efficiency and useful accuracy. DFT in the Kohn-Sham (KS) scheme (in the following

discussions, "DFT" means KS-DFT unless stated otherwise) simplifies a many-electron wavefunction problem to an auxiliary one-electron problem, delivering the ground-state energy and electron density in principle. But, in practice, its exchange-correlation part carrying the many-electron effect needs to be approximated. DFT with the local spin density approximation (LSDA) became popular in condensed matter physics, and then in quantum chemistry after generalized gradient approximations (GGAs) and hybrid GGAs were introduced. However, along with its success come the challenges to DFT (or TDDFT) [7], which include:

1. Estimation of fundamental band gaps (defined as $I - A$, where I is the ionization potential and A is the electron affinity) of semiconductors and insulators [7], and description for strongly-correlated electron systems [8] (e.g., Mott insulators), which are directly related to the derivative discontinuity of E_{xc} [8, 9].

2. Weak interactions (hydrogen bonds and van der Waals interactions), which are important for biological systems and soft condensed matter physics.

3. Applications of DFT to large or high-temperature systems, e.g., molecular dynamics simulations of liquids or warm dense matter.

4. Description for some excited states (e.g., Rydberg states, charge transfer states, double excitations, and conical intersection), and thus the calculation of spectroscopic observables of materials.

Many materials processes are closely related to these challenges. To illustrate this relation, I present here several examples that I am interested in. First is the carbon capture which requires finding materials that can selectively bind carbon dioxide molecules weakly such that CO_2 can be released easily and economically to be stored later. The Mg-MOF74 metal organic framework is one such material, in which CO2 binds to the MOF by the van der Waals interaction. The second example is the cathodic materials for lithium-ion batteries that are important for the information technology industry and the energy storage. The cathodic materials usually consist of transition metal oxides where d electrons are localized around transition metal ions and strongly correlated. Also, many cathodic materials are layered and bonded by weak interactions between layers. Another example is photovoltaic materials which are required to efficiently absorb light by having a band gap matching well the light spectrum, and to efficiently separate photoexcited electrons and holes.

While I am interested in the developments to tackle all these challenges, my current focuses are on the first two challenges and related applications, by starting from my work on meta-GGAs.

Advantages of Meta-GGAs

Meta-GGAs belong to a promising type of exchange-correlation approximations, that are potentially more accurate than GGAs but with comparable computational efficiency [1, 3], and thus are of special interest for large molecules, surfaces, and solids. Compared to GGAs, which use the electron density and its gradient as inputs, meta-GGAs add the kinetic energy density. Due to the semilocal feature of the kinetic energy density in computation, meta-GGAs are comparable to GGAs in terms of efficiency. Meanwhile, the inclusion of the electron kinetic energy density enables metaGGAs to recognize and accordingly treat different chemical bonds (e.g., covalent, metallic, and even weak bonds) that include the intermediate van der Waals interaction [1, 2, 3, 4]. Such performance cannot be obtained by a GGA [1, 3]. Meta-GGA could also serve as a better base for nonlocal functionals.

Developments and Applications of DFT (TDDFT) for Materials Research — A Research Agenda

1. *Development of a Meta-GGA for Band Gaps of Solids*

   Band gap is a fundamental property of materials that is of significant importance to other properties and their applications (e.g., topological insulating phases and the utilization of solar energy). However, the Kohn-Sham band gaps (defined as the energy difference of the lowest unoccupied orbital and the highest occupied orbital) of conventional semilocal density functionals are usually too small. Actually, even the exact exchange correlation functional would underestimate the KS band gap due to the existence of the derivative discontinuity of the exact V_{xc}. Nonlocal hybrid functionals that mix the nonlocal exact exchange with semilocal density functionals can improve the predictions, but with a dramatic sacrifice of the efficiency and thus not suitable for large systems. Many body perturbation theory can often provide more accurate and reliable predictions for band gaps, but it is even more computationally expensive than the hybrid functionals. Surprisingly, the SCAN band gaps are considerably larger than those from conventional semilocal density functionals. One of the reasons for the improvement is that metaGGAs are usually implemented in the manner of optimal variational effective potential, i.e., the total energies are optimized with respect to the orbitals, and therefore steps out the Kohn-Sham theorem. In view of the tremendous advantage in efficiency, it is very attractive to design a metaGGA for band gaps of solids. There have been studies trying to obtain accurate band gaps from semilocal functionals [10, 11]. Some encouraging progress has been made at the GGA level, but with a sacrifice of good description for total energies[11]. Since meta-GGAs have one more ingredient than GGAs, there is much room left for improvement of meta-GGAs.

2. *Development of Meta-GGA-based Nonlocal Functionals for Strongly-Correlated Electron Systems*

   Compounds involving transition metals are widely used in modern technologies due to their rich chemical and physical properties (e.g., catalytic, magnetic, and ferroelectric properties). However, theoretical descriptions of these compounds are usually difficult due to the near-degeneracy developed from the partially filled *d* subshells and the near-degenerate *(n+1)s* and *nd* subshells. The multi-reference feature resulted from the near-degeneracy makes inadequate wavefunction methods based on a single reference in quantum chemistry and the many body perturbation theory in condensed matter physics. DFT with semilocal approximations, on the other hand, does much better work on such systems. However, the performance of conventional semilocal approximations on transition metal compounds is usually not as good as that on the *sp* bonded systems, due to the presence of the nonlocal strong correlation originated from the near-degeneracy. Interestingly, from the preliminary results we have, SCAN improves the formation energies of solids with and without transiton metals significantly over the standard Perdew-Burke-Ernzehof (PBE) GGA. However, to fully address the strong correlation, nonlocal corrections have to be developed. Two approaches will be adopted.

   - Apply the Fermi-Orbital (FO) Perdew-Zunger (PZ) self-interaction correction (SIC) to meta-GGAs. The Perdew-Zunger self-interaction correction to GGAs usually improves performance on strongly-correlated (e.g., d- and f-electron) systems and band gaps, but worsens thermochemical properties of *sp* bonds. The FO-SIC on SCAN could solve this dilemma. This work will be conducted in collaboration with Profs. John Perdew and Mark Pederson.

- In the spirit of MGGA-MS and SCAN[2, 4] — which constructs a GGA for all 1- and 2-electron systems, and a GGA for slowly-varying densities, then interpolates between them through the right dimensionless parameter built from the kinetic energy density [3] — we replace the GGA with a nonlocal functional (e.g., one including exact exchange) for all 1- and 2-electron systems. Yang and his collaborators attributed many failures of DFT to the inability of the exchange-correlation approximations to treat accurately the stretched H_2 and H_2^+ molecules (one- and two-electron systems) simultaneously [8].

3. *Applications of DFT*

   With the excellent performance of SCAN and SCAN+vdW-correction, I will continue applying them to study the fundamental properties of 2D and layered materials as well as their applications for energy applications, which has been funded by the EFRC grant. Besides that, I am also interested in applying them to systems including (but not limited to) thermoelectric and ferroelectric materials as well as molecular crystals. The current priority will be given to the EFRC projects and the study on molecular crystals.

   - Mechanical, electronic, optical, and magnetic properties of the pristine and functionalized layered materials, and their potential applications for energy applications, will be studied theoretically and experimentally through the collaborations between the principal investigators of the DoE Energy Frontier Research Center (EFRC): Center for the Computational Design of Functional Layered Materials.
   - Molecular crystals play an important role in many areas of science ranging from mechanics and electronics to biology and medicine. They are crystalline solids that are composed of molecules bound together by relatively weak intermolecular interactions, typically consisting of vdW interactions and/or hydrogen bonds. A large amount of effort has been dedicated to understanding their structure and properties. Among them, an outstanding problem is polymorphism, which can have enormous effect on other properties of a crystal and is an active research area for pharmaceuticals, high energy materials, and dyes and pigments. Although the pair-wise vdW corrected conventional semilocal density functionals are reasonably accurate and widely applied for molecular crystals, distinguishing different polymorphs of a molecular crystal is still a difficult task. However, SCAN predicts the right energetic orders for the 4 water hexamer clusters and 7 ice polymorphs, which no previous density functional can do. This can be ascribed to the intermediate-range vdW interaction captured by SCAN, which is a true many-body effect missing in the pair-wise vdW corrected conventional semilocal approximations and is likely important in terms of distinguishing different polymorphs. Therefore, after adding the needed long-range vdW interaction, SCAN+vdW-correction can be useful for the study of polymorphism of molecular crystals.

4. *Screening for Minima of Reaction Space*

   In chemical reactions, identifications of reactants and products are of critical importance for thermodynamic and kinetic properties, with which the transition states between them can also be determined. We have devised a cheap way to screen for minima of reaction space of a molecular system, using the classical Coulomb energy of the system modeled by a collection of charged point ions to map out the ab initio potential energy surface determined by density functional theory. The method is reliable in identifying low-energy states of a manganese oxide cluster decorated

by water. I will extend this method to study catalytic problems, e.g., water splitting, methane oxidation, carbon monoxide oxidation, and hydrogenation and dehydrogenation using transition metal nanoparticles.

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TEACHING STATEMENT

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Teaching is an important part of my graduate training. I served as the Teaching Assistant for the course "Introductory Physics I Lab" for the 2008 academic year. This Teaching Assistant experience taught me the importance of being **patient** and **responsible** for students and how to be so. After the birth of my daughter on March 2011, the importance of these two characteristics become even clearer to me because great patience and responsibility are needed to teach a toddler who doesn't even know how to speak. As it turned out in that academic year, my teaching was successful and I was awarded 2008 Outstanding Teaching Assistant of the Year from American Association of Physics Teachers.

As a senior graduate student and postdoc fellow at Tulane University, I had opportunity to do substitute teaching on courses for graduate students, including Quantum Mechanics, Solid State Physics, and Atomic and Molecular Physics. Also, I was given an opportunity by Dr. James McGuire to teach undergraduate students for the first time as a guest lecturer in his class of "Introductory Physics" in Fall 2012. Kindly, the students gave honest and helpful advice for my teaching in cards after the class. This made me think that students are people, and teaching should be conducted in a respectful way. **Constructive communication** between teachers and students could result in resonance that benefits both.

After I moved to the Physics Department of Temple University as a Research Assistant Professor, I had a chance to teach a recitation of "elementary classical physics I" for about 120 students in 4 sections in Fall 2013. Unlike the previous experience, this class brought me more interactions with students and more thoughts about teaching. Generally, I think successful teaching involves three interacting components: **knowledge** by teaching new materials, **critical thinking** by asking questions about learned knowledge, and **curiosity** by questioning the limitations of learned knowledge which then drives them to acquire additional knowledge. However, the weight of each component should change according to the mission of a class and the background of the students in the class. In my recitation where students came for solutions of problems to test their knowledge, I put the priority on "critical thinking" and redelivering "knowledge". Since teaching is an **interactive** process, I also believe that a teacher needs to be **confident** in the class and accessible after class. A way to gain such confidence is by **preparing classes carefully**. Although the recitation only required me to solve the homework problems that were relatively easy, I went over the materials that the homework problems covered each time.

The courses I can teach at the undergraduate level include Introductory Physics (algebra-based), General Physics (calculus-based), Classical Mechanics, Modern Physics, Thermodynamics, Chemical Physics, and Computational Physics (or Computational Chemistry). At the graduate level, I can teach Quantum Mechanics, Solid State Physics/Chemistry, Atomic and Molecular Physics, and Molecular Quantum Mechanics. I am willing to learn to teach other subjects when needed.