

Mr. Shunhong Zhang (张顺洪)

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Education

- 2011.9 - present Ph. D. candidate, Mechanics (Advanced Materials and Mechanics)
Center for Applied Physics and Technology, Peking University
Department of Materials Science and Engineering, College of Engineering
Peking University (Supervisor: Professor Qian Wang)
- 2007.9 – 2011.7 Bachelor of Engineering (Engineering Structure Analysis)
Department of Mechanics and Engineering Science, College of Engineering
Peking University

Professional Experience

Research Assistant (2011.9 - present):

Participated actively in the following projects led by Prof. Qian Wang:

- NSFC: Computational design of new conductive materials based on non-metal light elements and investigations of their applications (2015.1-2018.12) (participated in writing the research proposal)
- NSFC: Simulations of 2D atomic sheets functionalized with superhalogens (2013.1-2014.12)
- NSFC: Design and modeling of 2p-electron based magnetic materials (2011.1-2015.12)
- National Grand Fundamental Research 973 Program of China: Novel quantum phenomenon induced by heterointerfaces and their manipulation (2012.1-2015.12)

Visiting Scholar (2014.3 - 2014.5):

Visited Professor Puru Jena's group, Department of Physics, Virginia Commonwealth University, VA, United States. (funded by the Graduate School of Peking University)

Peer Review (2015):

Serving as a reviewer for Journal of Applied Physics

Teaching Assistant (2012 - 2015):

for "Advanced Mathematics (D)" and "Computational Material Science and Engineering"

Research Interest:

I am interested in computational design of low-Z (light) element based new materials, especially low-dimensional materials, surfaces and interfaces, investigating their structural stability and phase transition, as well as the fundamental mechanical, electronic, and magnetic properties, and exploring their potential applications in nanomechanics, nanoelectronics, and spintronics.

Research Highlights:

- Computational design of 3D metallic carbon: published in *PNAS*, highlighted by *PNAS* blog, Physics Today etc.
- Computational design of metallic BN: published in *JACS*, highlighted by *JACS* spotlights, ChemistryViews etc.
- Computational design of pentagon based carbon sheet "penta-graphene": published in *PNAS*, highlighted by *PNAS* "in this issue"; reported by Chemistry World, Materials Today, etc.
- Computational modeling of the thermal exfoliation of single layer silica from the surface of Stishovite (001) thin film, published in *Nanoscale* and highlighted in the front cover.

Research Skills:

During my PhD studies I have been trained to skillfully use the standard density functional theory (DFT) based ab initio codes to perform electronic structure calculations, including VASP, Quantum ESPRESSO, Dmol3, CASTEP, Gaussian09, etc. In addition, I also got the hang of some more specialized packages, such as phonopy for phonon calculations, ShengBTE for phonon thermal transport, Wannier90 for mapping the electronic structure using maximally localized Wannier function, PythTB for tight binding band structure calculations, and LAMMPS for classic molecular dynamics simulations, etc. During research I have also combined standard ab initio methods with some statistical algorithms for multiscale simulations, for example, I have used the Monte Carlo simulation based on the Ising model to estimate the Curie temperature of ferromagnets, and implemented global optimization algorithms to search for stable or metastable crystal structures. I am familiar with coding using python, Fortran, and shell scripts.

Scholarships and Awards

2015	“Academic elites” for Graduates, Peking University
2015	Academic Top 10 (Rank No. 1), College of Engineering, Peking University
2015	IFSA scholarship, IFSA collaborative innovation center
2015	“Excellent paper” for the 3 rd PhD forum of College of Engineering, Peking University
2014 - 2015	Guanghua Scholarship, Peking University
2014 - 2015	Merit Student, Peking University
2014	Excellent poster prize, the 29 th annual meeting of Chinese Chemical Society
2013 - 2014	National Scholarship for Doctoral Students, Ministry of Education, P. R. China
2013 - 2016	The President’s Fellowship for Doctoral Students, Peking University
2012 - 2013	“Wusi” Scholarship, Peking University
2012 - 2015	Academic “Innovation Prize”, Peking University (three times)
2012	Schneider Scholarship, College of Engineering Peking University
2011	Sharp Scholarship, College of Engineering, Peking University
2010	Second Prize in “Jiang Zehan Cup” Mathematical Modeling and Computer Application Contest (Teammates: Mr. Kin Pang Cheong, Mr. Xu He)
2008 - 2009	Boeing Scholarship, Peking University
2008	Second Prize, the 25 th National Physics Contest of College Students
2006	Third Prize, the 23 rd National Physics Contest of High School Students

References

Professor Qian Wang, qianwang2@pku.edu.cn

Center for Applied Physics and Technology, Peking University

Professor Qiang Sun, sunqiang@pku.edu.cn

Department of Materials Science and Engineering, College of Engineering, Peking University

Professor Shaoqiang Tang, maotang@pku.edu.cn

Department of Mechanics and Engineering Science, College of Engineering, Peking University

Presentations

1. **Contributed talk:** *Structure, stability and properties modulation of stoichiometric graphene oxide.*
The 12th International Conference on Condensed Matter Theory and Computational Materials Science, Sun Yat-sen University, Guangzhou, China, Aug. 12 - Aug. 14, 2013.
(Partially Funded by the Graduate School of Peking University)
2. **Poster presentation:** *Robust ferromagnetism in monolayer chromium nitride.*
The 29th annual meeting of Chinese Chemical Society, Peking University, Beijing, China Aug. 3 - Aug. 7, 2014 (Excellent poster prize)
3. **Poster presentation:** *Strain induced topological phase transition in arsenene.*
International Symposium on Clusters and Nanomaterials (ISCAN) 2015, Richmond, VA, USA, Oct. 26 – Oct. 29, 2015. (Partially Funded by Graduate School of Peking University)

Publications

1. **S. Zhang**, J. Zhou, Q. Wang*, and P. Jena, Beyond graphitic carbon nitride: nitrogen-rich penta-CN₂ sheet. *J. Phys. Chem. C* **120**, 3993 (2016).
2. **S. Zhang**, J. Zhou, Q. Wang*, X. Chen, and P. Jena, Penta-graphene: A new carbon allotrope. *Proc. Natl. Acad. Sci. USA* **112**, 2372 (2015).
3. **S. Zhang**, Y. Li, T. Zhao, and Q. Wang*, Robust ferromagnetism in monolayer chromium nitride. *Sci. Rep.* **4**, 5241 (2014).
4. **S. Zhang**, Q. Wang*, Y. Kawazoe, and P. Jena, Three-dimensional metallic boron nitride. *J. Am. Chem. Soc.* **135**, 18216 (2013).
5. **S. Zhang**, Q. Wang*, X. Chen, and P. Jena, Stable three-dimensional metallic carbon with interlocking hexagons. *Proc. Natl. Acad. Sci. USA* **110**, 18809 (2013).
6. **S. Zhang**, J. Zhou, Q. Wang*, and Jena, P. Structure, stability, and property modulations of stoichiometric graphene oxide. *J. Phys. Chem. C* **117**, 1064 (2013).
7. **S. Zhang**, J. Zhou, X. Li, and Q. Wang*, Magnetism of triangular nanoflakes with different compositions and edge terminations. *J. Nanopart. Res.* **14**, 1171 (2012).
8. T. Zhao, **S. Zhang**, Y. Guo, and Q. Wang*, TiC₂: A New two-dimensional sheet beyond MXenes. *Nanoscale*, **8**, 233 (2016). (Highlighted on the Front Cover)
9. Y. Guo, **S. Zhang**, T. Zhao, and Q. Wang*, Thermal exfoliation of monolayer silica from bulk Stishovite phase. *Nanoscale* in press (2016). (Highlighted on the Front Cover)
10. X. Li, **S. Zhang**, F. Q. Wang, Y. Guo, J. Liu, and Q. Wang*, Tuning electronic and mechanical properties of penta-graphene via hydrogenation and fluorination. *Phys. Chem. Chem. Phys.* in press (2016) (Highlighted on the Front Cover)
11. J. Zhou, **S. Zhang**, Q. Wang, Y. Kawazoe, and P. Jena*, Self-assembly of metal atoms (Na, K, Ca) on graphene. *Nanoscale* **7**, 2352 (2015).
12. F. Q. Wang, **S. Zhang**, J. Yu, and Q. Wang*, Thermoelectric properties of single-layer SnSe. *Nanoscale*, **7**, 15962 (2015).
13. Y. Li, **S. Zhang**, J. Yu, Q. Wang, Q. Sun*, and P. Jena, A new C=C embedded porphyrin sheet with superior oxygen reduction performance. *Nano Res.* **8**, 2901 (2015). (*Nano Research paper of the Month Award*)
14. X. Li, **S. Zhang**, and Q. Wang*, Stability and physical properties of a tri-ring based

- porous $g\text{-C}_4\text{N}_3$ sheet. *Phys. Chem. Chem. Phys.* **15**, 7142 (2013).
15. Y. Li, **S. Zhang**, Q. Wang*, and P. Jena, Structure and properties of Mn_4Cl_9 : An antiferromagnetic binary hyperhalogen. *J. Chem. Phys.* **138**, 054309 (2013).
 16. Y. Guo, **S. Zhang**, and Q. Wang*, Electronic and optical properties of silicon based porous sheets. *Phys. Chem. Chem. Phys.* **16**, 16832 (2014).
 17. T. Zhao, **S. Zhang**, Q. Wang*, Y. Kawazoe, and P. Jena, Tuning the electronic and magnetic properties of silicene using magnetic superhalogen. *Phys. Chem. Chem. Phys.* **16**, 22979 (2014). (Highlighted on the Front Cover)
 18. M. Kan, J. Wang, X. Li, **S. Zhang**, Y. Li, Y. Kawazoe, Q. Sun*, and P. Jena, Structures and phase transition of a MoS_2 monolayer. *J. Phys. Chem. C* **118**, 1515 (2014).
 19. J. Liu, Y. Guo, **S. Zhang**, Q. Wang*, Y. Kawazoe, and P. Jena, New phosphorene allotropes containing ridges with 2- and 4-coordination. *J. Phys. Chem. C* **119**, 24674 (2015).
 20. J. Zhou, **S. Zhang**, Q. Wang, Q. Sun, and P. Jena, Coexistence of superconducting and large band gap quantum spin Hall effect in hafnium layer intercalated gallium film. Submitted. (2016)
 21. C. Zhang, **S. Zhang**, and Q. Wang*, Bonding-restricted structure search for novel 2D materials with dispersed C_2 dimers. Submitted. (2016)
 22. J. Liu, **S. Zhang**, Y. Guo, and Q. Wang*, Phosphorus K_4 crystal: a stable allotrope. In preparation. (2016)