

Peng Zhang, Ph.D

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Personal information:

Sex: Male

Nationality: Chinese

Date of Birth: Mar 1st, 1985

Marital status: Married

Education experience:

- Doctor of Philosophy, Materials Science & Engineering (Sep 2007 – Dec 2012)
Department of Materials Science and Engineering, Jilin University, China
Dissertation: Several Catalytic Processes on Fuel Cell Electrode Surface: A First Principles Study
Advisor: Prof. Qing Jiang
- Bachelor of Science, Materials Science & Engineering (Sep 2003 – Jun 2007)
Department of Materials Science and Engineering, Jilin University, China
Related courses: Chemistry, Physics, Chemicophysics, Materials Physics, Mechanics of Materials, Higher Mathematics, C Language, et al.

Work experience:

- Lecturer (Jan. 2013 - Sep. 2016)
School of Materials Science and Engineering, Jiangsu University, China
Course: Fundamentals of Materials Science and Engineering
- Association Professor (Sep. 2016 - Now)
School of Materials Science and Engineering, Jiangsu University, China
- Visiting Scholar (Nov. 2017 - now)
School of Physics, The University of Sydney, Australia

Research experience:

Investigated the mechanism of heterogeneous catalysis **by first-principles**

- Oxygen reduction reaction
 - Determined the potential dependent and structural selectivity of the oxygen reduction reaction on nitrogen-doped carbon nanotubes
 - Discovered the curvature effect of silicon-doped graphene and carbon nanotubes for oxygen reduction reaction
 - Detected the elemental dependent on the oxygen reduction activity of two-dimensional π -conjugated metal bis(dithiolene) complex nanosheets
- CO oxidation
 - Revealed the structural selectivity of CO oxidation on Fe/N/C catalysts
- CO₂ capture
 - Studied the curvature effect of CO₂ capture and reduction on SiC nanotubes

and sheets

Professional skills:

- Proficient in density functional theory and molecular dynamics calculations
- Familiar with many density functional theory and molecular dynamics codes, such as DMol3, CASTEP, Forcite and Discover
- Familiar with C language

Publications:

1. **P. Zhang**, B. B. Xiao, X. L. Hou, Y. F. Zhu,* Q. Jiang,* Layered SiC Sheets: A Potential Catalyst for Oxygen Reduction Reaction. *Sci. Rep.* 2014, 4, 3821.
2. **P. Zhang**, X. L. Hou, L. Liu, J. L. Mi,* M. D. Dong,* Two-Dimensional π -Conjugated Metal Bis(dithiolene) Complex Nanosheets as Selective Catalysts for Oxygen Reduction Reaction. *J. Phys. Chem. C* 2015, 119, 28028-28037.
3. **P. Zhang**, X. F. Chen, J. S. Lian, Q. Jiang,* Structure Selectivity of CO Oxidation on Fe/N/C Catalysts. *J. Phys. Chem. C* 2012, 116, 17572-17579.
4. **P. Zhang**, W. T. Zheng, Q. Jiang,* Behaviors of Monomer H₂O on the Cu(111) Surface under Surface Charges. *J. Phys. Chem. C* 2010, 114, 19331-19337.
5. **P. Zhang**, X. L. Hou,* J. L. Mi, Y. Q. He, L. Lin, Q. Jiang, M. D. Dong,* From Two-Dimension to One-Dimension: the Curvature Effect of Silicon-Doped Graphene and Carbon Nanotubes for Oxygen Reduction Reaction. *Phys. Chem. Chem. Phys.* 2014, 16, 17479-17486.
6. **P. Zhang**, J. S. Lian, Q. Jiang,* Potential Dependent and Structure Selectivity of the Oxygen Reduction Reaction on Nitrogen-Doped Carbon Nanotubes: A Density Functional Theory Study. *Phys. Chem. Chem. Phys.* 2012, 14, 11715-11723.
7. **P. Zhang**, X. L. Hou,* J. L. Mi, Q. Jiang, H. Aslanb, M. D. Dong,* Curvature Effect of SiC Nanotubes and Sheets for CO₂ Capture and Reduction. *RSC Adv.* 2014, 4, 48994-48999.
8. **P. Zhang**, Q. Hu, X. J. Yang, X. L. Hou,* J. L. Mi, L. Liu, M. D. Dong,* Size effect of oxygen reduction reaction on nitrogen-doped graphene quantum dots. *RSC Adv.* 2018, 8, 531-536.
9. **P. Zhang**, X. L. Hou,* J. L. Mi, L. Liu, M. D. Dong,* Oxygen Reduction Reaction on M-S4 Embedded Graphene: A Density Functional Theory Study. *Chem. Phys. Lett.* 2015, 641, 112-116.
10. **P. Zhang**, X. L. Hou,* S. Li, D. Liu, M. D. Dong,* Curvature Effect of O₂ Adsorption and Dissociation on SiC Nanotubes and Nanosheet. *Chem. Phys. Lett.* 2015, 619, 92-96.
11. **P. Zhang**,* X. L. Hou, Y. Q. He, Q. M. Peng,* M. D. Dong,* The Effects of Surface Group Functionalization and Strain on the Electronic Structures of Two-Dimensional Silicon Carbide. *Chem. Phys. Lett.* 2015, 628, 60-65.

12. X. L. Hou, **P. Zhang**,* S. Li, W. Liu,* Enhanced Electrocatalytic Activity of Nitrogen-Doped Olympicene/Graphene Hybrids for the Oxygen Reduction Reaction. *Phys. Chem. Chem. Phys.* 2016, 18, 22799-22804.
13. Y. Q. He, **P. Zhang**,* X. L. Hou, J. J. Xu, M. Q. Wang, Y. S. Wu, J. C. Qu, M. D. Dong,* Adjusting the Electronic Properties of Silicon Carbide Nanoribbons by Introducing Edge Functionalization. *RSC Adv.* 2014, 4, 35042-35047.
14. X. L. Hou, Q. Hu, **P. Zhang**,* J. Mi,* Oxygen Reduction Reaction on Nitrogen-Doped Graphene Nanoribbons: A Density Functional Theory Study. *Chem. Phys. Lett.* 2016, 663, 123-127.
15. C. He, **P. Zhang**, Y. F. Zhu, Q. Jiang,* Structures and Quantum Conduction of Copper Nanowires under Electric Fields using First Principles. *J. Phys. Chem. C* 2008, 112, 9045-9049.
16. B. B. Xiao, **P. Zhang**, L. P. Han, Z. Wen,* Functional MoS₂ by the Co/Ni Doping as the Catalyst for Oxygen Reduction Reaction, *Appl. Surf. Sci.* 2015, 354, 221-228.
17. H. Q. Feng, C. Y. Wu, **P. Zhang**, J. L. Mi,* M. D. Dong,* Facile Hydrothermal Synthesis and Formation Mechanisms of Bi₂Te₃, Sb₂Te₃ and Bi₂Te₃-Sb₂Te₃ Nanowires, *RSC Adv.* 2015, 5, 100309-100315.
18. H. Li,* S. Liu, L. Chen, J. Wu, **P. Zhang**, H. Tang, C. Li, X. Liu, Z. Wang, J. Meng,* Atomic Structures and Electronic Properties of Ta-doped 2H-NbSe₂, *RSC Adv.* 2014, 4, 57541-57546.