

Xiao ZHENG

Contact Information

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Personal Information

Sex: Male
Date of Birth: 10 March, 1980
Place of Birth: Fujian, China
Citizenship: PR China
Current position: Research Associate

Academic Experience

Postdoc (December, 2008 ~ to date)
Dept. of Chemistry, Duke University, USA
Supervisor: Prof. Weitao YANG
<http://www.chem.duke.edu/yang/index.htm>

Research Associate (January, 2007 ~ to date)
Dept. of Chemistry, Hong Kong University of Science and Technology, Hong Kong, China
Supervisor: Prof. YiJing YAN
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Education

Ph.D. in Theoretical Chemistry (September, 1998 ~ December, 2006)
Dept. of Chemistry, The University of Hong Kong, Hong Kong, China
Thesis title: "Quantum Mechanical Simulation of Open Electronic Systems"
Supervisor: Prof. GuanHua CHEN
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B.Sc. in Chemical Physics (September, 1998 ~ August, 2002)
University of Science and Technology of China, Hefei, Anhui, China

Research Interests

- First-principles method for open quantum systems and its application to nanoelectronics.
- Quantum mechanical simulation of complex systems.
- Development and implementation of quantum dissipation theory.
- Development and implementation of density functional theory.

Awards

- Outstanding Research Postgraduate Student Award (from The University of Hong Kong for the academic year 2005-2006).

Publications

1. “Numerical approach to time-dependent quantum transport and dynamical Kondo transition”, **Xiao Zheng**, Jinshuang Jin, and YiJing Yan, in preparation (2008).
2. “Equivalent electric circuit of two-terminal coherent electronic devices”, Yan Mo, GuanHua Chen, **Xiao Zheng**, and YiJing Yan, in preparation (2008).
3. “Complex non-Markovian effect on time-dependent quantum transport”, **Xiao Zheng**, JunYan Luo, Jinshuang Jin, and YiJing Yan, submitted (2008).
4. “Exact quantum dissipation theory for open many-electron systems: Hierarchical equations of motion approach”, Jinshuang Jin, **Xiao Zheng**, and YiJing Yan, submitted (2008).
5. “Dynamic Coulomb blockade in single-lead quantum dots”, **Xiao Zheng**, Jinshuang Jin, and YiJing Yan, *New J. Phys.* **10**, 093016 (2008).
6. “Dynamic electronic response of a quantum dot driven by time-dependent voltage”, **Xiao Zheng**, Jinshuang Jin, and YiJing Yan, *J. Chem. Phys.* **129**, 184112 (2008).
7. “Dynamic admittance of carbon nanotube-based molecular electronic devices and their equivalent electric circuit”, ChiYung Yam, Yan Mo, Fan Wang, Xiaobo Li, GuanHua Chen, **Xiao Zheng**, Yuki Matsuda, Jamil Tahir-Kheli, and William A. Goddard III, *Nanotechnology*, **19**, 495203 (2008).
8. “Exact dynamics of dissipative electronic systems and quantum transport: Hierarchical equations of motion approach”, Jinshuang Jin, **Xiao Zheng**, and YiJing Yan, *J. Chem. Phys.* **128**, 234703 (2008).
9. “The roles of apex dipoles and field penetration in the physics of charged, field emitting, single-walled carbon nanotubes”, Jie Peng, Zhibing Li, Chunshan He, Guihua Chen, Weiliang Wang, Shaozhi Deng, Ningsheng Xu, **Xiao Zheng**, GuanHua Chen, C. J. Edgcombe, and R. G. Forbes, *J. Appl. Phys.* **104**, 014310 (2008).
10. “First-principles method for open electronic systems”, **Xiao Zheng** and GuanHua Chen, *Nanoscale Phenomena: Basic Science to Device Application, Lecture Notes in Nanoscale Science and Technology*, Vol. 2, 235–243 (2007).
11. “Time-dependent density-functional theory for open systems”, **Xiao Zheng**, Fan Wang, ChiYung Yam, Yan Mo, and GuanHua Chen, *Phys. Rev. B* **75**, 195127 (2007).
12. “Maxwell’s demon and Smoluchowski’s trap door”, Jianzhou Zheng, **Xiao Zheng**, Yang Zhao, Yang Xie, ChiYung Yam, GuanHua Chen, Qing Jiang, and Allen T. Chwang, *Phys. Rev. E* **75**, 041109 (2007).
13. “Atomic decoration for improving the efficiency of field electron emission of carbon nanotubes”, Guihua Chen, Zhibing Li, Jie Peng, Chunshan He, Weiliang Wang, Shaozhi Deng, Ningsheng Xu, Chongyu Wang, Shanying Wang, **Xiao Zheng**, GuanHua Chen, and Tao Yu, *J. Phys. Chem. C* **111**, 4939 (2007).
14. “Some recent progresses in density-functional theory: efficiency, accuracy, and applicability”, ChiYung Yam, **Xiao Zheng**, and GuanHua Chen, *J. Comp. Theo. Nano.* **3**, 857 (2006).
15. “Effect of temperature on field emission from a micrometer-long single-walled carbon nanotube”, Chun-Sheng Wan, Zhen-Hua Li, Kang-Nian Fan, **Xiao Zheng**, and GuanHua Chen, *Phys. Rev. B* **73**, 165422 (2006).

16. "Quantum mechanical understanding of field dependence of the apex barrier of a single-wall carbon nanotube",
Jie Peng, Zhibing Li, Chunshan He, Shaozhi Deng, Ningsheng Xu, **Xiao Zheng**, and GuanHua Chen, *Phys. Rev. B* **72**, 235106 (2005).
17. "Linear-scaling quantum mechanical methods for nanoscopic structures",
ChiYung Yam, **Xiao Zheng**, and GuanHua Chen, *Handbook of Theoretical and Computational Nanotechnology*, edited by Michael Reith and Wolfram Schommers (American Scientific Publishers, California, 2005).
18. "A generalized exchange-correlation functional: the Neural Networks approach",
Xiao Zheng, LiHong Hu, XiuJun Wang, and GuanHua Chen, *Chem. Phys. Lett.* **390**, 186 (2004).
19. "Quantum mechanical investigation of field emission mechanism of a micrometer-long single-walled carbon nanotube",
Xiao Zheng, GuanHua Chen, Zhibing Li, Shaozhi Deng, and Ningsheng Xu, *Phys. Rev. Lett.* **92**, 106803 (2004).

Presentations

1. "Dynamic Coulomb blockade in single-lead quantum dots",
The Sixth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, 19~24 Jul, 2008.
2. "A first-principles method for open electronic systems",
231st American Chemical Society National Meeting, Atlanta, GA, U.S., 26~30 Mar, 2006.
3. "A first-principles method for open electronic systems",
The 9th National Quantum Chemistry Academic Conference, Guilin, China, 8~12 Oct, 2005.
4. "Quantum mechanical investigation of field emission mechanism of a micrometer-long single-wall carbon nanotube",
International workshop on theoretical and computational chemistry of complex systems in conjunction with 3rd Chinese theoretical and computational chemistry conference, Hong Kong, China, 3~7 Jan, 2005.
5. "Quantum mechanical investigation of field emission mechanism of a micrometer-long single-wall carbon nanotube",
Eleventh Symposium on Chemistry Postgraduate Research in Hong Kong, Hong Kong, China, 17 Apr, 2004.