Xiao Zheng

Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China
Tel: (86) 551-63600310 (O); Email: xz58@ustc.edu.cn
Web: http://staff.ustc.edu.cn/~xz58 | ResearchID | Google Scholar | ResearchGate

RESEARCH INTEREST

- Development of accurate and efficient density functional theory methods
- Development of theory for dissipative quantum systems
- Development of first-principles simulation methods for systems involving surfaces or interfaces, with applications to novel materials, nanoelectronics, photoenergy conversion, and strongly correlated systems
- Large-scale quantum mechanical simulation of complex systems

EDUCATION

2002–2006 **Ph.D. in Theoretical Chemistry**
Advisor: GuanHua Chen, Professor in Chemistry and Physics
Department of Chemistry, The University of Hong Kong, Thesis title: "*Quantum Mechanical Simulation of Open Electronic Systems*"

1998–2002 **B.Sc. in Chemistry**
Dept of Chemical Physics, University of Science and Technology of China

WORKING EXPERIENCE

Dec 2010 – Present **Associate Professor / Professor** (May 2015 – Present)
Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China

Dec 2008 – May 2011 **Visiting Scholar / Postdoctoral Research Associate**
Advisor: Weitao Yang, Philip Handler Professor of Chemistry
Department of Chemistry, Duke University

Jan 2007 – Dec 2009 **Postdoctoral Research Associate**
Advisor: YiJing Yan, Professor in Theoretical Chemistry
Dept of Chemistry, Hong Kong University of Science and Technology

AWARDS

1. Chinese Chemical Society Tang Ao-Qing Young Investigator Award in Theoretical Chemistry (2015, Chinese Chemical Society)

2. The National Science Fund for Excellent Young Scholars (2014, National Natural Science Foundation of China)
3. Outstanding Research Postgraduate Student Award (2005 – 2006, The University of Hong Kong)
4. Outstanding Undergraduate Scholarship (Annually in 1998 – 2002, University of Science and Technology of China)

SOFTWARE DEVELOPMENT

1. Main developer of **HEOM-QUICK** (USTC): A program which implements the hierarchical equations of motion method for strongly correlated open electronic systems
2. Co-developer of **LODESTAR** (HKU): A quantum chemistry software package which implements linear-scaling first-principles method for electronic structures, optical responses, and time-dependent quantum transport
3. Co-developer of **QM^{4}D** (Duke): A quantum mechanical/molecular mechanical molecular dynamics simulation package with a broad range of applications

ACADEMIC SERVICES

1. Editorial Board Member of *New Journal of Physics*, (May 2020 – Present)

PUBLICATIONS IN PEER--REVIEWED JOURNALS

1. Lyuzhou Ye, Longqing Yang, **Xiao Zheng**[*], and Shaul Mukamel, "Enhancing circular dichroism signals with vector beams", *Phys. Rev. Lett.* accepted (2021).
2. Yao Wang[*], Yu Su, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan, "Marcus' electron transfer rate revisited via a Rice-Ramsperger-Kassel-Marcus analogue: A unified formalism for linear and nonlinear solvation scenarios", *Chin. J. Chem. Phys.* 10.1063/1674-0068/cjcp2101004 (2021).
3. Xiao-Long Zhang[†], Peng-Peng Yang[†], Ya-Rong Zheng, Yu Duan, Shao-Jin Hu, Tao Ma, Fei-Yue Gao, Zhuang-Zhuang Niu, Zhi-Zheng Wu, Shuai Qin, Li-Ping Chi, Xingxing Yu, Rui Wu, Chao Gu, Cheng-Ming Wang, Xu-Sheng Zheng, **Xiao Zheng**, Jun-Fa Zhu, and Min-Rui Gao[*], "An efficient turing-type Ag_2Se-$CoSe_2$ multi-interfacial oxygen-evolving electrocatalyst", *Angew. Chem. Int. Ed.* 10.1002/anie.202017016 (2021).
4. Hou-Ming Xu[†], Chao Gu[†], Xiao-Long Zhang[†], Lei Shi, Qiang Gao, Shaojin Hu, Shi-Kui Han[*], **Xiao Zheng**, Min-Rui Gao[*], and Shu-Hong Yu[*], "Phase-controlled 1T transition-metal dichalcogenide-based multidimensional hybrid nanostructures", *CCS Chem.* **3**, 58-68 (2021).
5. Xiangzhong Zeng, Lyuzhou Ye, Daochi Zhang, Rui-Xue Xu, **Xiao Zheng**[*], and Massimiliano Di Ventra[*], "Effect of quantum resonances on local temperature in nonequilibrium open systems", *Phys. Rev. B* **103**, (8), 085411 (2021).
6. Huanhuan Liu[†], Jia Lei[†], Shangjie Yang, Fengfeng Qin, Lei Cui, Yuan Kong[*], **Xiao Zheng**, Tao Duan, Wenkun Zhu[*], and Rong He[*], "Boosting the oxygen evolution

activity over cobalt nitride nanosheets through optimizing the electronic configuration", *Appl. Catal. B* **286**, 119894 (2021).

7. Xiaolong Yang, **Xiao Zheng**[*], and Weitao Yang[*], "Density functional prediction of quasiparticle, excitation, and resonance energies of molecules with a global scaling correction approach", *Front. Chem.* **8**, 588808 (2020).
8. Hong Gong[†], Yao Wang[†], Hou-Dao Zhang, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan[*], "Thermodynamic free-energy spectrum theory for open quantum systems", *J. Chem. Phys.* **153**, (21), 214115 (2020).
9. Hong Gong[†], Yao Wang[†], Hou-Dao Zhang[*], Qin Qiao, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan[*], "Equilibrium and transient thermodynamics: A unified dissipaton-space approach", *J. Chem. Phys.* **153**, (15), 154111 (2020).
10. Xiangyang Li[†], Liang Zhu[†], Bin Li, Jingcheng Li, Pengfei Gao, Longqing Yang, Aidi Zhao, Yi Luo, Jianguo Hou, **Xiao Zheng**[*], Bing Wang[*], and Jinlong Yang[*], "Molecular molds for regularizing Kondo states at atom/metal interfaces", *Nat. Commun.* **11**, (1), 2566 (2020).
11. Arif Ullah, Lu Han, Yun-An Yan, **Xiao Zheng**[*], YiJing Yan, and Vladimir Chernyak, "Stochastic equation of motion approach to fermionic dissipative dynamics. II. Numerical implementation", *J. Chem. Phys.* **152**, (20), 204106 (2020).
12. Lu Han, Arif Ullah, Yun-An Yan, **Xiao Zheng**[*], YiJing Yan, and Vladimir Chernyak, "Stochastic equation of motion approach to fermionic dissipative dynamics. I. Formalism", *J. Chem. Phys.* **152**, (20), 204105 (2020).
13. Fuzhen Bi, ChiYung Yam, Chengjie Zhao, Le Liu, Min Zhao, **Xiao Zheng**, and Tonggang Jiu[*], "Enhanced photocurrent in heterostructures formed between $CH_3NH_3PbI_3$ perovskite films and graphdiyne", *Phys. Chem. Chem. Phys.* **22**, (11), 6239-6246 (2020).
14. Hou-Dao Zhang[†], Lei Cui[†], Hong Gong, Rui-Xue Xu, **Xiao Zheng**[*], and YiJing Yan, "Hierarchical equations of motion method based on Fano spectrum decomposition for low temperature environments", *J. Chem. Phys.* **152**, (6), 064107 (2020).
15. Fei-Yue Gao[†], Shao-Jin Hu[†], Xiao-Long Zhang, Ya-Rong Zheng, Hui-Juan Wang, ZhuangZhuang Niu, Peng-Peng Yang, Rui-Cheng Bao, Tao Ma, Zheng Dang, Yong Guan, Xu-Sheng Zheng, **Xiao Zheng**, Jun-Fa Zhu, Min-Rui Gao[*], and Shu-Hong Yu[*], "High-curvature transition metal chalcogenide nanostructures with a pronounced proximity effect enable fast and selective CO_2 electroreduction", *Angew. Chem. Int. Ed.* **59**, (22), 8706-8712 (2020), DOI: 10.1002/anie.201912348.
16. Xiaolong Yang, Zhouyi He, and **Xiao Zheng**[*], "Unit cell consistency of maximally localized Wannier functions", *Electron. Struct.* **2**, (1), 014001 (2020).
17. Longqing Yang, Xiaoli Wang, Faiza Uzma, **Xiao Zheng**[*], and YiJing Yan, "Evolution of magnetic anisotropy of an organometallic molecule in a mechanically controlled break junction: The roles of connecting electrodes", *J. Phys. Chem. C* **123**, (50), 30754-30764 (2019).
18. Xiao-Long Zhang[†], Shao-Jin Hu[†], Ya-Rong Zheng[†], Rui Wu, Fei-Yue Gao, Peng-Peng Yang, Zhuang-Zhuang Niu, Chao Gu, Xingxing Yu, Xu-Sheng Zheng, Cheng

Ma, **Xiao Zheng**, Jun-Fa Zhu, Min-Rui Gao*, and Shu-Hong Yu*, "Polymorphic cobalt diselenide as extremely stable electrocatalyst in acidic media via a phase-mixing strategy", *Nat. Commun.* **10**, 5338 (2019).

19. Yu Duan†, Zi-You Yu†, Shao-Jin Hu†, Xu-Sheng Zheng, Chu-Tian Zhang, Hong-He Ding, Bi-Cheng Hu, Qi-Qi Fu, Zhi-Long Yu, **Xiao Zheng**, Jun-Fa Zhu, Min-Rui Gao*, and Shu-Hong Yu*, "Scaled-up synthesis of amorphous NiFeMo oxides and their rapid surface reconstruction for superior oxygen evolution catalysis", *Angew. Chem. Int. Ed.* **58**, (44), 15772-15777 (2019).
20. Daochi Zhang, **Xiao Zheng***, and Massimiliano Di Ventra, "Local temperatures out of equilibrium", *Phys. Rep.* **830**, 1-66 (2019).
21. Lu Han, Vladimir Chernyak, Yun-An Yan, **Xiao Zheng***, and YiJing Yan, "Stochastic representation of non-Markovian fermionic quantum dissipation", *Phys. Rev. Lett.* **123**, (5), 050601 (2019).
22. Lei Cui, Hou-Dao Zhang*, **Xiao Zheng***, Rui-Xue Xu, and YiJing Yan, "Highly efficient and accurate sum-over-poles expansion of Fermi and Bose functions at near zero temperatures: Fano spectrum decomposition scheme", *J. Chem. Phys.* **151**, (2), 024110 (2019).
23. Rulin Wang, Wencai Lu, Hang Xie*, **Xiao Zheng**, and ChiYung Yam*, "Theoretical investigation of real-time charge dynamics in open systems coupled to bulk materials", *J. Chem. Phys.* **150**, (17), 174119 (2019).
24. Yao He†, Bo Zhang†, Hao Dong*, Penglin Xu, Xiaoying Cai, Ting Zhou, Mu Yu, Jun Liang, **Xiao Zheng***, and Changlin Tian*, "Equilibria between the K^+ binding and cation vacancy conformations of potassium channels", *Protein & Cell* **10**, (7), 533-537 (2019).
25. Fuzhen Bi, **Xiao Zheng**, and ChiYung Yam*, "First-principles study of mixed cation methylammonium-formamidinium hybrid perovskite", *Acta Phys.-Chim. Sin.* **35**, 69–75 (2019). DOI: 10.3866/PKU.WHXB201801082.
26. **Xiao Zheng***, "Precise simulation of strongly correlated quantum impurity systems (in Chinese)", *Chin. Sci. Bull.* **63**, DOI: 10.1360/N972018-0089 (2018).
27. Yu Wang*, Xiaoguang Li*, **Xiao Zheng**, and Jinlong Yang, "Manipulation of spin and magnetic anisotropy in bilayer magnetic molecular junctions", *Phys. Chem. Chem. Phys.* **20**, 26396 (2018). DOI: 10.1039/c8cp05759a.
28. ZhenHua Li, YongXi Cheng, JianHua Wei*, **Xiao Zheng**, and YiJing Yan, "Kondo-peak splitting and resonance enhancement caused by inter-dot tunneling in coupled double quantum dots", *Phys. Rev. B* **98**, 115133 (2018). DOI: 10.1103/PhysRevB.98.115133.
29. Hong Gong, Arif Ullah, LvZhou Ye, **Xiao Zheng***, and YiJing Yan, "Quantum entanglement of parallel-coupled double quantum dots: A theoretical study using the hierarchical equations of motion approach", *Chin. J. Chem. Phys.* **31**, 510 (2018). DOI:10.1063/1674-0068/31/cjcp1806138.
30. Lu Han, Hou-Dao Zhang, **Xiao Zheng***, and YiJing Yan, "On the exact truncation tier of fermionic hierarchical equations of motion", *J. Chem. Phys.* **148**, 234108 (2018). DOI: 10.1063/1.5034776.

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32. Xiaoli Wang, Longqing Yang, LvZhou Ye, **Xiao Zheng***, and YiJing Yan, "Precise control of local spin states in an adsorbed magnetic molecule with an STM tip: Theoretical insights from first-principles-based simulation", *J. Phys. Chem. Lett.* **9**, 2418−2425 (2018). DOI: 10.1021/acs.jpclett.8b00808.
33. Hou-Dao Zhang*, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan*, "Statistical quasi-particle theory for open quantum systems", *Mol. Phys.* **116**, 780-812 (2018). DOI: 10.1080/00268976.2018.1431407.
34. Chao Gu†, Shaojin Hu†, Xusheng Zheng†, Min-Rui Gao*, Ya-Rong Zheng, Lei Shi, Qiang Gao, **Xiao Zheng**, Wangsheng Chu, Hong-Bin Yao, Junfa Zhu, and Shu-Hong Yu*, "Synthesis of sub-2 nm iron-doped $NiSe_2$ nanowires and their surface-confined oxidation for oxygen evolution catalysis", *Angew. Chem. Int. Ed.* **57**, 4020-4024 (2018). DOI: 10.1002/anie.201800883.
35. Chen Li, **Xiao Zheng**, Neil Qiang Su, and Weitao Yang*, "Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations", *Natl. Sci. Rev.* **5**, 203-215 (2018). DOI: 10.1093/nsr/nwx111.
36. DaDi Zhang, Xiaolong Yang, **Xiao Zheng***, and Weitao Yang*, "Accurate density functional prediction of molecular electron affinity with the scaling corrected Kohn–Sham frontier orbital energies", *Mol. Phys.* **116**, 927-934 (2018). DOI: 10.1080/00268976.2017.1382738.
37. Qin Liu, JingChun Wang, PengLi Du, LiHong Hu, **Xiao Zheng***, and GuanHua Chen, "Improving the performance of long-range-corrected exchange-correlation functional with an embedded neural network", *J. Phys. Chem. A* **121**, 7273-7281 (2017).
38. Yu Wang*, Xiaoguang Li, **Xiao Zheng**, and Jinlong Yang, "Spin switch in iron phthalocyanine on Au(111) surface by hydrogen adsorption", *J. Chem. Phys.* **147**, 134701 (2017).
39. Yuan Kong, Dong Hou, Hou-Dao Zhang*, **Xiao Zheng**, and Rui-Xue Xu*, "Davydov collective vibrational modes and infrared spectrum features in aniline crystal: Influence of geometry change induced by Van der Waals interactions", *J. Phys. Chem. C* **121**, 18867-18875 (2017).
40. LvZhou Ye, Hou-Dao Zhang*, Yao Wang, **Xiao Zheng***, and YiJing Yan, "Low-frequency logarithmic discretization of the reservoir spectrum for improving the efficiency of hierarchical equations of motion approach", *J. Chem. Phys.* **147**, 074111 (2017).
41. Hou-Dao Zhang*, Qin Qiao, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan, "Efficient steady-state solver for hierarchical quantum master equations", *J. Chem. Phys.* **147**, 044105 (2017).
42. Fuzhen Bi, Stanislav Markov, Rulin Wang, YanHo Kwok, Weijun Zhou, Limin Liu, **Xiao Zheng**, GuanHua Chen, and ChiYung Yam*, "Enhanced photovoltaic

properties induced by ferroelectric domain structures in organometallic halide perovskites", *J. Phys. Chem. C* **121**, 11151-11158 (2017).

43. ZhenHua Li, JianHua Wei, **Xiao Zheng**, YiJing Yan, and Hong-Gang Luo*, "Corrected Kondo temperature beyond the conventional Kondo scaling limit", *J. Phys.: Condens. Matter* **29**, 175601 (2017).
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45. Jin-Jin Ding, Yao Wang, Hou-Dao Zhang*, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan*, "Fokker–Planck quantum master equation for mixed quantum–semiclassical dynamics", *J. Chem. Phys.* **146**, 024104 (2017).
46. Penglin Xu, Ting Zhou, Nadia Natalia, Shaojin Hu, and **Xiao Zheng***, "Rational ligand design for an efficient biomimetic water splitting complex", *J. Phys. Chem. A* **120**, 10033-10042 (2016).
47. LvZhou Ye, **Xiao Zheng***, YiJing Yan, and Massimiliano Di Ventra*, "Thermodynamic meaning of local temperature of nonequilibrium open quantum systems", *Phys. Rev. B* **94**, 245105 (2016).
48. Jin-Jin Ding*, Hou-Dao Zhang*, Yao Wang, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan*, "Minimum-exponents ansatz for molecular dynamics and quantum dissipation", *J. Chem. Phys.* **145**, 204110 (2016).
49. LvZhou Ye, Xiaoli Wang, Dong Hou, Rui-Xue Xu, **Xiao Zheng***, and YiJing Yan, "HEOM-QUICK: a program for accurate, efficient, and universal characterization of strongly correlated quantum impurity systems", *WIREs Comput. Mol. Sci.* **6**, 608 (2016), doi: 10.1002/wcms.1269.
50. Yu Wang, **Xiao Zheng***, and Jinlong Yang*, "Kondo screening and spin excitation in few-layer CoPc molecular assembly stacking on Pb(111) surface: A DFT+HEOM study", *J. Chem. Phys.* **145**, 154301 (2016).
51. Tian-min Wu, Rui-Xue Xu, **Xiao Zheng***, and Wei Zhuang*, "Electronic structures and thermoelectric properties of two-dimensional MoS_2/$MoSe_2$ heterostructures", *Chin. J. Chem. Phys.* **29**, 445 (2016).
52. Pu Huang, Jingwei Zhou, Liang Zhang, Dong Hou, Shaochun Lin, Wen Deng, Chao Meng, Changkui Duan, Chenyong Ju, **Xiao Zheng**, Fei Xue, and Jiangfeng Du*, "Generating giant and tunable nonlinearity in a macroscopic mechanical resonator from a single chemical bond", *Nat. Commun.* **7**, 11517 (2016).
53. YiJing Yan*, Jinshuang Jin, Rui-Xue Xu, and **Xiao Zheng**, "Dissipaton equation of motion approach to open quantum systems", *Front. Phys.* **11**, 110306 (2016).
54. Yu Wang, **Xiao Zheng***, and Jinlong Yang*, "Environment-modulated Kondo phenomena in FePc/Au(111) adsorption systems", *Phys. Rev. B* **93**, 125114 (2016).
55. Xiaoli Wang, Dong Hou*, **Xiao Zheng***, and YiJing Yan, "Anisotropy induced Kondo splitting in a mechanically stretched molecular junction: A first-principles based study", *J. Chem. Phys.* **144**, 034101 (2016).

56. **Xiao Zheng***, Chen Li, Dadi Zhang, and Weitao Yang*, "Scaling correction approaches for reducing delocalization error in density functional approximations", *Sci. China Chem.* **58**, 1825-1844 (2015), invited review.
57. Rui-Xue Xu*, Hou-Dao Zhang, **Xiao Zheng**, and YiJing Yan*, "Dissipaton equation of motion for system-and-bath interference dynamics", *Sci. China Chem.* **58**, 1816-1824 (2015), invited review.
58. Jinshuang Jin, Shikuan Wang, **Xiao Zheng**, and YiJing Yan*, "Current noise spectra and mechanisms with dissipaton equation of motion theory", *J. Chem. Phys.* **142**, 234108 (2015).
59. LvZhou Ye, Dong Hou, **Xiao Zheng***, YiJing Yan, and Massimiliano Di Ventra*, "Local temperatures of strongly-correlated quantum dots out of equilibrium", *Phys. Rev. B* **91**, 205106 (2015).
60. DaDi Zhang, **Xiao Zheng***, Chen Li, and Weitao Yang*, "Orbital relaxation effects on Kohn–Sham frontier orbital energies in density functional theory", *J. Chem. Phys.* **142**, 154113 (2015).
61. RuLin Wang, **Xiao Zheng***, YanHo Kwok, Hang Xie, GuanHua Chen, and ChiYung Yam*, "Time-dependent density functional theory for open systems with a positivity-preserving decomposition scheme for environment spectral functions", *J. Chem. Phys.* **142**, 144112 (2015).
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63. Zhong-Gang Liu, Yu-Feng Sun, Wen-Kai Chen, Yuan Kong, Zhen Jin, Xing Chen, **Xiao Zheng***, Jin-Huai Liu, Xing-Jiu Huang*, and Shu-Hong Yu*, "Facet-dependent stripping behavior of Cu_2O microcrystals toward lead ions: A rational design for the determination of lead ions", *Small* 11, 2493-2498 (2015). DOI: 10.1002/smll.201402146 (cover paper).
64. Chen Li, **Xiao Zheng***, Aron J. Cohen, Paula Mori-Sánchez, and Weitao Yang*, "Local scaling correction for reducing delocalization error in density functional approximations", *Phys. Rev. Lett.* **114**, 053001 (2015).
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69. Dong Hou, Rulin Wang, **Xiao Zheng**[*], NingHua Tong[*], JianHua Wei, and YiJing Yan[*], "Hierarchical equations of motion for an impurity solver in dynamical mean-field theory", *Phys. Rev. B* 90, 045141 (2014).
70. **Xiao Zheng**[*] and Rulin Wang, "Time-dependent density-functional theory for open electronic systems", *Sci. China Chem.* **57**, 26 (2014) invited review.
71. Yan Ho Kwok, Hang Xie, Chi Yung Yam, **Xiao Zheng**, and GuanHua Chen[*], "Time-dependent density functional theory quantum transport simulation in non-orthogonal basis", *J. Chem. Phys.* **139**, 224111 (2013).
72. Rulin Wang, Dong Hou, and **Xiao Zheng**[*], "Time-dependent density-functional theory for real-time electronic dynamics on material surfaces", *Phys. Rev. B* **88**, 205126 (2013).
73. Hang Xie[*], Yanho Kwok, Yu Zhang, Feng Jiang, **Xiao Zheng**, YiJing Yan, and GuanHua Chen[*], "Time-dependent quantum transport theory and its application to graphene nanoribbons", *Phys. Status Solidi B* **250**, 2481 (2013).
74. JianQiao Zhang, ZhenYu Yin, **Xiao Zheng**, ChiYung Yam, and GuanHua Chen[*], "Gauge-invariant and current-continuous microscopic ac quantum transport theory", *Eur. Phys. J. B* **86**, 423 (2013).
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81. ZhenHua Li, NingHua Tong, **Xiao Zheng**[*], Dong Hou, JianHua Wei[*], Jie Hu, and YiJing Yan[*], "Hierarchical Liouville-space approach for accurate and universal characterization of quantum impurity systems", *Phys. Rev. Lett.* **109**, 266403 (2012).
82. **Xiao Zheng**[*], Min Liu, Erin R. Johnson[*], Julia Contreras-García, and Weitao Yang[*], "Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains", *J. Chem. Phys.* **137**, 214106 (2012).
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transport: An efficient method based on Liouville-von-Neumann equation for single-electron density matrix", *J. Chem. Phys.* **137**, 044113 (2012).

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95. **Xiao Zheng***, Jinshuang Jin, Sven Welack, Meng Luo, and YiJing Yan*, "Numerical approach to time-dependent quantum transport and dynamical Kondo transition", *J. Chem. Phys.* **130**, 164708 (2009).
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PROCEEDINGS AND BOOK CHAPTERS

110. Lei Cui, RulinWang, ChiYung Yam, GuanHua Chen, and **Xiao Zheng**[*], "Quantum mechanical simulation of electron dynamics on surfaces of materials",

Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile, *Springer Series in Materials Science*, Vol. **284**, 115-136 (2021).

111. Jinshuang Jin, **Xiao Zheng**, and YiJing Yan*, "Dissipative dynamic theory for open many-electron systems: Hierarchical equations-of-motion approach", *AIP Conference Proceedings: Solid-state quantum computing* **1074**, 96 (2008).
112. **Xiao Zheng** and GuanHua Chen*, "First-principles method for open electronic systems", *Nanoscale Phenomena: Basic Science to Device Application, Lecture Notes in Nanoscale Science and Technology*, Vol. **2**, 235-243 (2007).
113. ChiYung Yam, **Xiao Zheng**, and GuanHua Chen*, "Linear-scaling quantum mechanical methods for nanoscopic structures", *Handbook of Theoretical and Computational Nanotechnology*, edited by Michael Reith and Wolfram Schommers (American Scientific Publishers, California, 2005).

CONFERENCE PRESENTATIONS

1. "Quantum Dissipative Dynamics in Low Temperature and Strong Coupling Regime", *2020 Workshop on Computational and Statistical Mechanics in Complex Systems*, Hangzhou (online), China, December 2020.
2. "Strong electron correlation from the perspective of open quantum systems", *Workshop on New Methods for Strongly Correlated Electrons*, Qingdao, October 2019.
3. "Strongly correlated open electronic systems: Theories and applications", *Inaugural Workshop at Qingdao Institute for Theoretical and Computational Sciences*, Qingdao, August 2019.
4. "Precise control of local quantum states in adsorbed magnetic molecules: Insights from first-principles-based simulations", *The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)*, Hong Kong, July 2019.
5. "Strongly correlated open electronic systems: Theories and applications", *2019 Telluride Workshop on "Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy"*, Telluride, CO, USA, July 2019.
6. "Improving density functional calculations for molecular band gaps and electron affinities", *KITS Workshop on Frontiers in DFT and Beyond – Advances and Challenges*, Beijing, May 2019.
7. "Precise control of local quantum states in adsorbed magnetic molecules: Insights from first-principles-based simulations", *Symposium on "Electronic Structure and Dynamics of Complex Systems"*, Beijing, April 2019.
8. "Precise control of quantum states in adsorbed magnetic molecules: Insights from first-principles-based simulations", *The 4th Graduate Symposium on Chemistry and Materials Science at USTC*, Hefei, November 2018.
9. "Theoretical investigation on the control of local spin states in adsorbed magnetic molecules", *2018 Spin Mini Workshop: Exotic magnetic phenomena*, Chengdu, June 2018.

10. "Recent Progress in HEOM and SEOM methods for fermionic open quantum systems", *2018 Workshop on Hierarchical and Stochastic Schrödinger Equations*, Xiamen, May 2018.
11. "Theoretical investigation on the control of local quantum states in adsorbed magnetic molecules", *31st Chinese Chemical Society Annual Meeting (Session 20: Quantum and Classical Dynamics)*, Hangzhou, May 2018.
12. "Improving the density functional calculation on molecular electron affinities", *31st Chinese Chemical Society Annual Meeting (Session 21: Electronic Structure Theories and Methods)*, Hangzhou, May 2018.
13. "Theoretical investigation on the control of local quantum states in adsorbed magnetic molecules", *2018 Workshop on Electronic Structure Theories and Methods for Young Researchers*, Xiamen, March 2018.
14. "Theoretical investigations on local quantum states in single molecules adsorbed on metal surfaces", *The 14th National Workshop on Computers in Chemistry*, Nanjing, China, November 2017.
15. "Controlling quantum states in adsorbed molecular magnets: First-principles based studies", *International Workshop on Quantum Systems in Chemistry, Physics and Biology (QSCP-XXII)*, Changsha, China, October 2017.
16. "Local temperature and local heating in nonequilibrium quantum dot systems", *Telluride Workshop on "Energy Transport in Nanoscale Gaps and Molecular Junctions"*, Telluride, CO, USA, July 2017.
17. "An accurate and universal hierarchical dynamics approach to open quantum systems", *The 3rd China-Japan-Korea Workshop on Theoretical and Computational Chemistry*, Daejeon, Republic of Korea, Jan 2017.
18. "Control of quantum states in adsorbed single molecular magnets", *2016 Workshop on Computational and Statistical Mechanics in Complex Systems*, Shenzhen, China, Nov 2016.
19. "Accurate simulation of single molecular magnets adsorbed on metal surfaces", *Workshop for Chinese Young Physical Chemists*, Dalian, China, Nov 2016.
20. "First-principles based characterization of local electronic states in adsorbed single molecular magnets: DFT+HEOM approach", *7th Cross-Strait Theoretical and Computational Chemistry Conference*, Changsha, China, Oct 2016.
21. "Theoretical investigations on strong electron correlation effects in magnetic molecules adsorbed on material surfaces", *30th Chinese Chemical Society Annual Meeting*, Dalian, China, Jul 2016.
22. "Local temperatures of quantum impurity systems out of equilibrium", *7th Asia-Pacific Conference of Theoretical and Computational Chemistry*, Kaohsiung, Taiwan, Jan 2016.
23. "Accurate and universal hierarchical dynamics approach to strongly correlated quantum impurity systems", *CECAM Workshop on Open Quantum Systems: Computational Methods*, Hong Kong, China, Dec 2015.
24. "Local temperatures of open systems out of equilibrium", *2015 Workshop on Computational and Statistical Mechanics in Complex Systems*, Beijing, China, Oct 2015.

25. "Local temperatures of quantum impurity systems out of equilibrium", *Workshop on Nonequilibrium Processes in Small Systems 2015*, Guiyang, China, July 2015.
26. "First-principles simulation of real-time electronic dynamics on surfaces of materials", *Progress in Electromagnetics Research Symposium 2015*, Prague, Czech Republic, July 2015.
27. "Hierarchical equations of motion method for strongly correlated electronic systems", *Recent Advances in Quantum Dynamics and Thermodynamics of Complex Systems 2015*, Beijing, China, Jun 2015.
28. "Hierarchical equations of motion method for quantum transport and quantum control", *Workshop on Frontiers of Quantum Information*, Hangzhou, China, May 2015.
29. "A hierarchical dynamics approach to strongly correlated quantum impurity systems", *Workshop on Quantum Simulation*, Hong Kong, China, Dec 2014.
30. "First-principles method for electronic dynamics on surfaces of materials", *Workshop on Computational Materials and Computational Biology*, Hong Kong, China, Nov 2014.
31. "A hierarchical dynamics approach to strongly correlated quantum impurity systems", *XIXth International Workshop on Quantum Systems in Chemistry, Physics and Biology*, Tamsui, Taiwan, Nov 2014.
32. "Improving the accuracy of density functional approximations", *2014 Workshop on Computational and Statistical Mechanics in Complex Systems*, Changchun, China, Sep 2014.
33. "A scaling correction approach to density functional approximations", *2nd Chinese Young Chemical Physicists Forum*, Guiyang, China, Aug 2014.
34. "An accurate and universal HEOM approach to strongly correlated quantum impurity systems", *2014 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry*, Quzhou, China, Aug 2014.
35. "Applications of a hierarchical dynamics approach to quantum dissipation and quantum control", *Workshop on Quantum Dissipation and Quantum Control*, Lanzhou, China, Apr 2014.
36. "TDDFT for open systems", *Hong Kong Spring School on Quantum Simulation Methods*, Hong Kong, China, Apr 2014.
37. "A hierarchical dynamics approach and its applications to strongly correlated electronic systems", *International Conference on Computational Modeling Methods and Applications*, Changchun, China, Sept 2013.
38. "A hierarchical dynamics approach and applications to strongly correlated systems and real-time electronic dynamics", *Telluride Workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy"*, Telluride CO, USA, July 2013.
39. "First principles method for complex open quantum systems and its applications", *Workshop for Chinese Young Physical Chemists*, Hangzhou, China, Apr 2013.
40. "Hierarchical dynamics approach to strongly correlated quantum impurity systems, and electronic dynamics at surfaces", *Workshop on Computational Methods for Complex Systems (CMCS 2012)*, Hong Kong, China, Dec 2012.

41. "Quantum mechanical methods for open systems: Theories and applications", *Workshop on Computational Statistical Mechanics of Complex Systems 2012*, Hefei, China, Oct 2012.
42. "First-principles methods for time-dependent quantum transport", *5th Workshop on Theories of Electron Transport and Simulation of Nanoelectronic Devices*, Xi'an, China, Sep 2012.
43. "Quantum mechanical methods for open systems: Theories and applications", *1st Chinese Young Chemical Physicists Forum*, Guiyang, China, Jul 2012.
44. "Quantum Liouville-space approach to strongly correlated quantum impurity systems", *International Conference on Theoretical and High Performance Computational Chemistry 2012*, Nanjing, China, Jul 2012.
45. "Hiearchical equations of motion approach to strongly correlated quantum impurity systems", *Workshop on Quantum Information, Quantum Dissipation and Associated Physics 2012*, Chengdu, China, Jun 2012.
46. "Improving band gap prediction in density functional theory from molecules to solids", *28th Chinese Chemical Society Annual Meeting*, Chengdu, China, Apr 2012.
47. "Improving band gap prediction in density functional theory from molecules to solids", *243rd American Chemical Society National Meeting*, San Diego, CA, USA, Mar 2012.
48. "Transient electronic dynamics in strongly correlated systems: Hierarchical equations of motion approach", *CECAM Workshop on simulation and modeling of emerging electronics (SMEE 2011)*, Hong Kong, China, Dec 2011.
49. "Hierarchical equations of motion method for strongly correlated systems", *Workshop on computational and statistical mechanics for complex systems*, Chengdu, China, Sep 2011.
50. "First principles simulation of time-dependent quantum transport: Dynamic admittance and equivalent circuit", *Workshop on simulation and modeling of emerging electronics (SMEE 2010)*, Hong Kong, China, Dec 2010.
51. "Improving band gap prediction by density functional theory: From atoms to solids", *240th American Chemical Society National Meeting*, Boston, MA, USA, Aug 2010.
52. "Exact real-time dynamics of electron transport in mesoscopic systems", *American Physical Society March Meeting 2009*, Pittsburgh, PA, USA, Mar 2009.
53. "Dynamic Coulomb blockade in single-lead quantum dots", *The Sixth Congress of the International Society for Theoretical Chemical Physics* (*ISTCP-VI*), Vancouver, Canada, Jul 2008.
54. "A first-principles method for open electronic systems", *231st American Chemical Society National Meeting*, Atlanta, GA, USA, Mar 2006.
55. "A first-principles method for open electronic systems", *The Ninth National Quantum Chemistry Academic Conference*, Guilin, China, Oct 2005.
56. "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, Jan 2005.

57. "Quantum mechanical investigation of field emission mechanism of a micrometer-long single-wall carbon nanotube", *The 11th Symposium on Chemistry Postgraduate Research in Hong Kong*, Hong Kong, China, Apr 2004.

OTHER INVITED TALKS

58. "Precise control of local quantum states in adsorbed molecular magnets: Insights from first-principles-based simulations", Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Nov 2019.
59. "Strong electron correlation from the perspective of open quantum systems", New York University Shanghai, Shanghai, Nov 2019.
60. "Precise control of local quantum states in adsorbed magnetic molecules: First-principles-based studies", Hangzhou Normal University, Hanzhou, Apr 2019.
61. "A scaling correction approach for improving density functional approximations", Beijing Normal University, Beijing, China, Jun 2015.
62. "A hierarchical dynamics approach for open quantum systems, and its application to strongly correlated electronic systems", Beijing Computational Science Research Center, Beijing, China, Nov 2013.
63. "Hierarchical dynamics approach to strongly correlated quantum impurity systems and electronic dynamics on surfaces", East China Normal University, Shanghai, China, Jan 2013.
64. "Introduction to quantum mechanics of open systems", *2012 Summer school for graduate students "Theoretical Chemistry"*, Guangzhou, China, Aug 2012.
65. "Hierarchical equations of motion approach to strongly correlated quantum impurity systems", Guizhou Normal College, Guiyang, China, Apr 2012.
66. "Simulation and design of next-generation nanoelectronic devices from first principles", Guizhou Normal College, Guiyang, China, Apr 2012.

CONFERENCE ORGANIZATION

1. Workshop on Statistical Dynamics of Complex Systems, Hefei, China, Apr 2015.
2. Workshop on Computational Statistical Mechanics of Complex Systems 2012, Hefei, China, Oct 2012.