

Xiao Zheng

Department of Chemistry, Fudan University, Shanghai 200433, China

Tel: (+86) 18255148511; Email: xzheng@fudan.edu.cn

Web: [Google Scholar](#) | [ResearchGate](#)

RESEARCH INTEREST

- Fundamental theories for open quantum systems
- Accurate, efficient and universal methods for many-body open quantum systems
- Novel theoretical methods leveraging artificial intelligence and quantum computing technologies
- Electronic structure theories from an open systems perspective
- Applications to nanoelectronics, spintronics, thermoelectrics, optical spectroscopy, catalysis, spin sensing and control, strongly correlated 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**

Department of Chemical Physics, University of Science and Technology of China

WORKING EXPERIENCE

Mar 2022 – **Professor**

Present Department of Chemistry, Fudan University

Dec 2010 – **Associate Professor / Professor** (from May 2014)

Feb 2022 Hefei National Laboratory for Physical Sciences at the Microscale &
Department of Chemical Physics, University of Science and Technology of China

Dec 2008 – **Visiting Scholar / Postdoctoral Research Associate**

May 2011 Advisor: Weitao Yang, Philip Handler Professor of Chemistry
Department of Chemistry, Duke University

Jan 2007 – **Postdoctoral Research Associate**

Dec 2009 Advisor: YiJing Yan, Professor in Theoretical Chemistry
Department 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 & Fudan): 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 **QM⁴D** (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. **Xiao Zheng**, GuanHua Chen*, Zhibing Li, Shaozhi Deng, and Ningsheng Xu*, “Quantum mechanical investigation of field emission mechanism of a micrometer-long single-walled carbon nanotube”, *Phys. Rev. Lett.* **92**, (10), 106803 (2004).
2. **Xiao Zheng**, LiHong Hu, XiuJun Wang, and GuanHua Chen*, “A generalized exchange-correlation functional: the Neural Networks approach”, *Chem. Phys. Lett.* **390**, (1-3), 186-192 (2004).
3. Jie Peng, Zhibing Li, Chunshan He, Shaozhi Deng, Ningsheng Xu*, **Xiao Zheng**, and GuanHua Chen*, “Quantum mechanical understanding of field dependence of the apex barrier of a single-wall carbon nanotube”, *Phys. Rev. B* **72**, (23), 235106 (2005).
4. Chun-Sheng Wan, Zhen-Hua Li, Kang-Nian Fan*, **Xiao Zheng**, and GuanHua Chen*, “Effect of temperature on field emission from a micrometer-long single-walled carbon nanotube”, *Phys. Rev. B* **73**, (16), 165422 (2006).
5. ChiYung Yam, **Xiao Zheng**, and GuanHua Chen*, “Some recent progresses in density-functional theory: efficiency, accuracy, and applicability”, *J. Comput. Theor. Nanosci.* **3**, (5), 857-863 (2006).
6. 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, “Atomic decoration for improving the efficiency of field electron emission of carbon nanotubes”, *J. Phys. Chem. C* **111**, (13), 4939-4945 (2007).
7. Jianzhou Zheng, **Xiao Zheng**, Yang Zhao*, Yang Xie, ChiYung Yam, GuanHua Chen*, Qing Jiang, and Allen T. Chwang, “Maxwell’s demon and Smoluchowski’s trap door”, *Phys. Rev. E* **75**, (4), 041109 (2007).
 8. **Xiao Zheng**, Fan Wang, ChiYung Yam, Yan Mo, and GuanHua Chen*, “Time-dependent density-functional theory for open systems”, *Phys. Rev. B* **75**, (19), 195127 (2007).
 9. 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, “The roles of apex dipoles and field penetration in the physics of charged, field emitting, single-walled carbon nanotubes”, *J. Appl. Phys.* **104**, (1), 014310 (2008).
 10. Jinshuang Jin, **Xiao Zheng**, and YiJing Yan*, “Exact dynamics of dissipative electronic systems and quantum transport: Hierarchical equations of motion approach”, *J. Chem. Phys.* **128**, (23), 234703 (2008).
 11. ChiYung Yam, Yan Mo, Fan Wang, Xiaobo Li, GuanHua Chen*, **Xiao Zheng***, Yuki Matsuda, Jamil Tahir-Kheli, and William A. Goddard III*, “Dynamic admittance of carbon nanotube-based molecular electronic devices and their equivalent electric circuit”, *Nanotechnology* **19**, (49), 495203 (2008).
 12. **Xiao Zheng***, Jinshuang Jin, and YiJing Yan*, “Dynamic electronic response of a quantum dot driven by time-dependent voltage”, *J. Chem. Phys.* **129**, (18), 184112 (2008).
 13. **Xiao Zheng**, Jinshuang Jin, and YiJing Yan*, “Dynamic Coulomb blockade in single-lead quantum dots”, *New J. Phys.* **10**, 093016 (2008).
 14. **Xiao Zheng***, JunYan Luo, Jinshuang Jin, and YiJing Yan*, “Complex non-Markovian effect on time-dependent quantum transport”, *J. Chem. Phys.* **130**, (12), 124508 (2009).
 15. **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**, (16), 164708 (2009).
 16. Yan Mo, **Xiao Zheng***, GuanHua Chen, and YiJing Yan, “Transient electronic dynamics of noninteracting open systems beyond linear response”, *J. Phys.: Condens. Matter* **21**, (35), 355301 (2009).
 17. **Xiao Zheng**, San-Huang Ke*, and Weitao Yang*, “Conductive junctions with parallel graphene sheets”, *J. Chem. Phys.* **132**, (11), 114703 (2010).
 18. Jianzhou Zheng, **Xiao Zheng**, ChiYung Yam, and GuanHua Chen*, “Computer simulation of Feynman’s ratchet and pawl system”, *Phys. Rev. E* **81**, (6), 061104 (2010).
 19. **Xiao Zheng**, GuanHua Chen*, Yan Mo, SiuKong Koo, Heng Tian, ChiYung Yam, and YiJing Yan*, “Time-dependent density functional theory for quantum transport”, *J. Chem. Phys.* **133**, (11), 114101 (2010).
 20. Shizheng Wen, SiuKong Koo, ChiYung Yam*, **Xiao Zheng***, YiJing Yan, Zhongmin Su, Kangnian Fan, Li Cao, Wenping Wang, and GuanHua Chen*,

- “Time-dependent current distributions of a two-terminal carbon nanotube-based electronic device”, *J. Phys. Chem. B* **115**, (18), 5519-5525 (2011).
21. ChiYung Yam, **Xiao Zheng**, GuanHua Chen, Yong Wang, Thomas Frauenheim, and Thomas A. Niehaus*, “Time-dependent versus static quantum transport simulations beyond linear response”, *Phys. Rev. B* **83**, (24), 245448 (2011).
 22. **Xiao Zheng***, ChiYung Yam, Fan Wang, and GuanHua Chen*, “Existence of time-dependent density-functional theory for open electronic systems: Time-dependent holographic electron density theorem”, *Phys. Chem. Chem. Phys.* **13**, (32), 14358-14364 (2011).
 23. Eugenia S. Tam, Joshua J. Parks, William W. Shum, Yu-Wu Zhong, Mitk’El B. Santiago-Berríos, **Xiao Zheng**, Weitao Yang, Garnet K.-L. Chan, Héctor D. Abruna, and Daniel C. Ralph*, “Single-molecule conductance of pyridine-terminated dithienylethene switch molecules”, *ACS Nano* **5**, (6), 5115-5123 (2011).
 24. **Xiao Zheng**, Aron J. Cohen, Paula Mori-Sánchez, Xiangqian Hu, and Weitao Yang, “Improving band gap prediction in density functional theory from molecules to solids”, *Phys. Rev. Lett.* **107**, (2), 026403 (2011).
 25. Siu Kong Koo, ChiYung Yam*, **Xiao Zheng**, and GuanHua Chen, “First-principles Liouville-von Neumann equation for open systems and its applications”, *Phys. Status Solidi B* **249**, (2), 270-275 (2012).
 26. **Xiao Zheng**, Rui-Xue Xu, Jian Xu, Jinshuang Jin, Jie Hu, and YiJing Yan*, “Hierarchical equations of motion for quantum dissipation and quantum transport”, *Prog. Chem.* **24**, (6), 1129-1152 (2012).
 27. Hang Xie, Feng Jiang, Heng Tian, **Xiao Zheng**, Yanho Kwok, Shuguang Chen, ChiYung Yam, YiJing Yan, and GuanHua Chen*, “Time-dependent quantum transport: An efficient method based on Liouville-von-Neumann equation for single-electron density matrix”, *J. Chem. Phys.* **137**, (4), 044113 (2012).
 28. **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**, (21), 214106 (2012).
 29. 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**, (26), 266403 (2012).
 30. Ting Zhou, Xiangsong Lin, and **Xiao Zheng***, “First-principles study on structural and chemical asymmetry of a biomimetic water-splitting dimanganese complex”, *J. Chem. Theory Comput.* **9**, (2), 1073-1080 (2013).
 31. Lei Wang†, Wei-Hong Xu†, Ran Yang, Ting Zhou, Dong Hou, **Xiao Zheng***, Jin-Huai Liu, and Xing-Jiu Huang*, “Electrochemical and density functional theory investigation on high selectivity and sensitivity of exfoliated nano-zirconium phosphate toward lead (II)”, *Anal. Chem.* **85**, (8), 3984-3990 (2013).
 32. **Xiao Zheng***, Ting Zhou, and Weitao Yang*, “A nonempirical scaling correction approach for density functional methods involving substantial amount of Hartree-Fock exchange”, *J. Chem. Phys.* **138**, (17), 174105 (2013).

33. Shikuan Wang, **Xiao Zheng**^{*}, Jinshuang Jin, and YiJing Yan^{*}, “Hierarchical Liouville-space approach to nonequilibrium dynamical properties of quantum impurity systems”, *Phys. Rev. B* **88**, (3), 035129 (2013).
34. **Xiao Zheng**, YiJing Yan, and Massimiliano Di Ventra, “Kondo memory in driven strongly correlated quantum dots”, *Phys. Rev. Lett.* **111**, (8), 086601 (2013).
35. Qingping Zhang, **Xiao Zheng**^{*}, Jun Jiang, and Wei Liu^{*}, “Structural stability of $\text{La}_2\text{Ce}_2\text{O}_7$ as a proton conductor: A first-principles study”, *J. Phys. Chem. C* **117**, (40), 20379-20386 (2013).
36. 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**, (10), 423 (2013).
37. Hang Xie^{*}, Yanho Kwok, Yu Zhang, Feng Jiang, **Xiao Zheng**, YiJing Yan, and GuanHua Chen^{*}, “Time-dependent quantum transport theory and its applications to graphene nanoribbons”, *Phys. Status Solidi B* **250**, (11), 2481-2494 (2013).
38. Rulin Wang, Dong Hou, and **Xiao Zheng**^{*}, “Time-dependent density-functional theory for real-time electronic dynamics on material surfaces”, *Phys. Rev. B* **88**, (20), 205126 (2013).
39. 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**, (22), 224111 (2013).
40. **Xiao Zheng**^{*} and Rulin Wang, “Time-dependent density-functional theory for open electronic systems”, *Sci. China Chem.* **57**, (1), 26-35 (2014), invited review.
41. 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**, (4), 045141 (2014).
42. Yu Wang, **Xiao Zheng**^{*}, Bin Li, and Jinlong Yang^{*}, “Understanding the Kondo resonance in the d-CoPc/Au(111) adsorption system”, *J. Chem. Phys.* **141**, (8), 084713 (2014).
43. LvZhou Ye, Dong Hou, Rulin Wang, Dewen Cao, **Xiao Zheng**^{*}, and YiJing Yan^{*}, “Thermopower of few-electron quantum dots with Kondo correlations”, *Phys. Rev. B* **90**, (16), 165116 (2014).
44. Hang Xie^{*}, Yanho Kwok, Feng Jiang, **Xiao Zheng**, and GuanHua Chen^{*}, “Complex absorbing potential based Lorentzian fitting scheme and time dependent quantum transport”, *J. Chem. Phys.* **141**, (16), 164122 (2014).
45. Hou-Dao Zhang, Rui-Xue Xu^{*}, **Xiao Zheng**, and YiJing Yan^{*}, “Nonperturbative spin–boson and spin–spin dynamics and nonlinear Fano interferences: A unified dissipaton theory based study”, *J. Chem. Phys.* **142**, (2), 024112 (2015).
46. 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**, (5), 053001 (2015).
47. 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**, (21), 2493-2498 (2015). DOI: 10.1002/smll.201402146 (cover paper).
48. Dong Hou, Shikuan Wang, Rulin Wang, LvZhou Ye, RuiXue Xu, **Xiao Zheng**^{*}, and YiJing Yan^{*}, “Improving the efficiency of hierarchical equations of motion approach and application to coherent dynamics in Aharonov-Bohm interferometers”, *J. Chem. Phys.* **142**, (10), 104112 (2015).
 49. 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**, (14), 144112 (2015).
 50. 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**, (15), 154113 (2015).
 51. 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**, (20), 205106 (2015).
 52. Jinshuang Jin[†], Shikuan Wang[†], **Xiao Zheng**, and YiJing Yan^{*}, “Current noise spectra and mechanisms with dissipaton equation of motion theory”, *J. Chem. Phys.* **142**, (23), 234108 (2015).
 53. 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**, (12), 1816-1824 (2015), invited review, doi: 10.1007/s11426-015-5499-2
 54. **Xiao Zheng**^{*}, Chen Li, Dadi Zhang, and Weitao Yang^{*}, “Scaling correction approaches for reducing delocalization error in density functional approximations”, *Sci. China Chem.* **58**, (12), 1825-1844 (2015), invited review, doi: 10.1007/s11426-015-5501-z.
 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**, (3), 034101 (2016).
 56. Yu Wang, **Xiao Zheng**^{*}, and Jinlong Yang^{*}, “Environment-modulated Kondo phenomena in FePc/Au(111) adsorption systems”, *Phys. Rev. B* **93**, (12), 125114 (2016).
 57. YiJing Yan^{*}, Jinshuang Jin, Rui-Xue Xu, and **Xiao Zheng**, “Dissipaton equation of motion approach to open quantum systems”, *Front. Phys. China* **11**, (4), 110306 (2016).
 58. 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).
 59. Tian-min Wu, Rui-Xue Xu, **Xiao Zheng**^{*}, and Wei Zhuang^{*}, “Electronic structures and thermoelectric properties of two-dimensional MoS₂/MoSe₂ heterostructures”, *Chin. J. Chem. Phys.* **29**, (4), 445-452 (2016).

60. 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**, (15), 154301 (2016).
61. 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**, (6), 608-638 (2016), doi: 10.1002/wcms.1269.
62. 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**, (20), 204110 (2016).
63. LvZhou Ye, **Xiao Zheng**^{*}, YiJing Yan, and Massimiliano Di Ventra^{*}, “Thermodynamic meaning of local temperature of nonequilibrium open quantum systems”, *Phys. Rev. B* **94**, (24), 245105 (2016).
64. 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**, (50), 10033-10042 (2016).
65. 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**, (2), 024104 (2017).
66. Kaiqi Wu[†], Wenfei Li[†], Lu Yu[†], Wei Tong, Yue Feng, Shenglong Ling, Longhua Zhang, **Xiao Zheng**^{*}, Maojun Yang^{*}, and Changlin Tian^{*}, “Temperature-dependent ESR and computational studies on antiferromagnetic electron transfer in the yeast NADH dehydrogenase Ndi1”, *Phys. Chem. Chem. Phys.* **19**, (6), 4849-4854 (2017).
67. 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**, (17), 175601 (2017).
68. 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**, (21), 11151-11158 (2017).
69. 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**, (4), 044105 (2017).
70. 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**, (7), 074111 (2017).
71. 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**, (34), 18867-18875 (2017).
72. 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**, (13), 134701 (2017).

73. 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**, (38), 7273-7281 (2017).
74. 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**, (7-8), 927-934 (2018).
75. Hou-Dao Zhang^{*}, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan^{*}, “Statistical quasi-particle theory for open quantum systems”, *Mol. Phys.* **116**, (7-8), 780-812 (2018).
76. 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**, (2), 203-215 (2018).
77. 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 NiSe₂ nanowires and their surface-confined oxidation for oxygen evolution catalysis”, *Angew. Chem. Int. Ed.* **57**, (15), 4020-4024 (2018).
78. 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**, (9), 2418–2425 (2018).
79. Penglin Xu, Shaojin Hu, Hou-Dao Zhang^{*}, and **Xiao Zheng**^{*}, “Theoretical insights into the reactivity of Fe-based catalysts for water oxidation: the role of electron-withdrawing groups”, *Phys. Chem. Chem. Phys.* **20**, (21), 14919-14926 (2018).
80. 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**, (23), 234108 (2018). DOI: 10.1063/1.5034776
81. 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**, (4), 510-516 (2018). Invited paper for the special issue for celebration of “The 60th Anniversary of University of Science and Technology of China and the 30th Anniversary of Chinese Journal of Chemical Physics”.
82. 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**, (11), 115133 (2018).
83. 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**, (41), 26396-26404 (2018).
84. **Xiao Zheng**^{*}, “Precise simulation of strongly correlated quantum impurity systems (in Chinese)”, *Chin. Sci. Bull.* **63**, (33), 3412-3418 DOI: 10.1360/N972018-0089 (2018).

85. Fuzhen Bi, **Xiao Zheng**, and ChiYung Yam*, “First-principles study of mixed cation methylammonium-formamidinium hybrid perovskite”, *Acta Phys.-Chim. Sin.* **35**, (1), 69-75 (2019).
86. 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).
87. 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).
88. 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).
89. 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).
90. Daochi Zhang, **Xiao Zheng***, and Massimiliano Di Ventra, “Local temperatures out of equilibrium”, *Phys. Rep.* **830**, 1-66 (2019).
91. 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).
92. 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).
93. 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).
94. Xiaolong Yang, Zhouyi He, and **Xiao Zheng***, “Unit cell consistency of maximally localized Wannier functions”, *Electron. Struct.* **2**, (1), 014001 (2020).
95. 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 CO₂ electroreduction”, *Angew. Chem. Int. Ed.* **59**, (22), 8706-8712 (2020), DOI: 10.1002/anie.201912348.
96. 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). DOI: 10.1063/1.5136093
97. Fuzhen Bi, ChiYung Yam, Chengjie Zhao, Le Liu, Min Zhao, **Xiao Zheng**, and Tonggang Jiu*, “Enhanced photocurrent in heterostructures formed between CH₃NH₃PbI₃ perovskite films and graphdiyne”, *Phys. Chem. Chem. Phys.* **22**, (11), 6239-6246 (2020). DOI: 10.1039/d0cp00170h
98. 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). DOI: 10.1063/1.5142164
99. 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). DOI: 10.1063/1.5142166
100. 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).
101. Hong Gong[†], Yao Wang[†], Hou-Dao Zhang*, Qin Qiao, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan*, “Equilibrium and transient thermodynamics: A unified dissipation-space approach”, *J. Chem. Phys.* **153**, (15), 154111 (2020).
102. 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).
103. 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).
104. 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).
105. 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).
106. 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).
107. 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 Ag₂Se-CoSe₂ multi-interfacial oxygen-evolving electrocatalyst”, *Angew. Chem. Int. Ed.* **60**, (12), 6553-6560 (2021). DOI:10.1002/anie.202017016

108. 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.* **34**, (4), 462-470 (2021). DOI:10.1063/1674-0068/cjcp2101004
109. Lyuzhou Ye, Longqing Yang, **Xiao Zheng***, and Shaul Mukamel, “Enhancing circular dichroism signals with vector beams”, *Phys. Rev. Lett.* **126**, (12), 123001 (2021). DOI: 10.1103/PhysRevLett.126.123001
110. Faiza Uzma, Longqing Yang, Dawei He, Xiaoli Wang, Shaojin Hu, Lyuzhou Ye*, **Xiao Zheng***, and YiJing Yan, “Understanding the sub-meV-precision tuning of magnetic anisotropy of single-molecule junction”, *J. Phys. Chem. C* **125**, (12), 6990-6997 (2021).
111. Shaojin Hu, Penglin Xu, Rui-Xue Xu, and **Xiao Zheng***, “Unveiling the high catalytic activity of a dinuclear iron complex for the oxygen evolution reaction”, *Inorg. Chem.* **60**, (10), 7297-7305 (2021).
112. Rulin Wang*, Fuzhen Bi, Wencai Lu, **Xiao Zheng**, and ChiYung Yam*, “Tracking electron dynamics of single molecules in scanning tunneling microscopy junctions with laser pulses”, *J. Phys. Chem. Lett.* **12**, (27), 6398-6404 (2021). DOI: 10.1021/acs.jpcclett.1c01293
113. Jianfei Sui, Hang Liu, Shaojin Hu, Kang Sun, Gang Wan, Hua Zhou, **Xiao Zheng**, and Hai-Long Jiang*, “A general strategy to immobilize single-atom catalysts in metal-organic frameworks for enhanced photocatalysis”, *Adv. Mater.* 2109203 (2021). DOI: 10.1002/adma.202109203
114. Xiangyang Li, Hong Gong, Qingfeng Zhuang, Bing Wang, **Xiao Zheng***, and Jinlong Yang*, “Reaction on a rink: Kondo-enhanced heterogeneous single-atom catalysis”, *J. Phys. Chem. C* **125**, 21488-21495 (2021).
115. Daochi Zhang, Xu Ding, Hou-Dao Zhang, **Xiao Zheng***, and YiJing Yan, “Adiabatic terminator for fermionic hierarchical equations of motion”, *Chin. J. Chem. Phys.* **34**, 905 (2021). DOI:10.1063/1674-0068/cjcp2110212
116. Lei Cui, DaDi Zhang*, Yuan Kong*, and **Xiao Zheng**, “CO₂ reduction on metal-doped SnO₂(110) surface catalysts: Manipulating the product by changing the ratio of Sn:O”, *Chin. J. Chem. Phys.* **35**, 413 (2022). DOI:10.1063/1674-0068/cjcp2104077
117. Zhi-Zheng Wu†, Xiao-Long Zhang†, Zhuang-Zhuang Niu†, Fei-Yue Gao, Peng-Peng Yang, Li-Ping Chi, Lei Shi, Wen-Sen Wei, Ren Liu, Zhi Chen, Shaojin Hu, **Xiao Zheng**, and Min-Rui Gao*, “Identification of Cu(100)/Cu(111) interfaces as superior active sites for CO dimerization during CO₂ electroreduction”, *J. Am. Chem. Soc.* **144**, 259-269 (2022). DOI:10.1021/jacs.1c09508
118. Yan-Ru Wang†, Qing-Feng Zhuang†, Yi Li, Ya-Lin Hu, Yang-Yi Liu*, Qiao-Bao Zhang, Lei Shi, Chuan-Xin He, **Xiao Zheng**, and Shu-Hong Yu*, “Bio-inspired synthesis of transition-metal oxide hybrid ultrathin nanosheets for enhancing the cycling stability in lithium-ion batteries”, *Nano Research* **15**, 5064-5071 (2022). DOI:10.1007/s12274-021-4030-7

119. XiongZhi Zeng, Wei Hu, **Xiao Zheng**, Jin Zhao, Zhenyu Li*, and Jinlong Yang*, “Computational characterization of nanosystems”, *Chin. J. Chem. Phys.* **35**, 1 (2022). DOI:10.1063/1674-0068/cjcp2111233
120. JingChun Wang, DaDi Zhang, Rui-Xue Xu, ChiYung Yam, GuanHua Chen, and **Xiao Zheng***, “Improving density functional prediction of molecular thermochemical properties with a machine-learning-corrected generalized gradient approximation”, *J. Phys. Chem. A* **126**, (6), 970-978 (2022). DOI:10.1021/acs.jpca.1c10491
121. YongXi Cheng, ZhenHua Li*, **Xiao Zheng**, JianHua Wei*, Hong-Gang Luo*, Hai-Qing Lin, and YiJing Yan, “Magnetic field dependent Kondo transport through double quantum dots system”, *Ann. Phys. (Berlin)* 2100439 (2022). DOI:10.1002/andp.202100439
122. Qingfeng Zhuang†, Xiaoli Wang†, Lyuzhou Ye*, YiJing Yan, and **Xiao Zheng***, “Origin of asymmetric splitting of Kondo peak in spin-polarized scanning tunneling spectroscopy: Insights from first-principles-based simulations”, *J. Phys. Chem. Lett.* **13**, (9), 2094-2100 (2022). DOI:10.1021/acs.jpcllett.2c00228
123. ZhenHua Li, YongXi Cheng, **Xiao Zheng**, JianHua Wei, YiJing Yan, and Hong-Gang Luo*, “Study the mixed valence problem in asymmetric Anderson model: Fano-Kondo resonance around Fermi level”, *J. Phys.: Condens. Matter* **34**, 255601 (2022). DOI: 10.1088/1361-648X/ac640a
124. Yan-Ru Wang†, Qingfeng Zhuang†, Rui Cao†, Yi Li, Fei-Yue Gao, Zhao-Rui Li, Zhen He, Lei Shi, Yu-Feng Meng, Xu Li, Jin-Long Wang, Yu Duan, Min-Rui Gao, **Xiao Zheng**, and Shu-Hong Yu*, “Reduction-controlled atomic migration for single atom alloy library”, *Nano Lett.* **22**, 4232-4239 (2022). DOI: 10.1021/acs.nanolett.2c01314
125. Zi-Hao Chen, Yao Wang, **Xiao Zheng**, Rui-Xue Xu, and YiJing Yan*, “Universal time-domain Prony fitting decomposition for optimized hierarchical quantum master equations”, *J. Chem. Phys.* **156**, 221102 (2022). DOI: 10.1063/5.0095961
126. Yao Wang*, Zi-Hao Chen, Rui-Xue Xu, **Xiao Zheng**, and YiJing Yan*, “A statistical quasi-particles thermofield theory with Gaussian environments: System-bath entanglement theorem for nonequilibrium correlation functions”, *J. Chem. Phys.* **157**, 044102 (2022). DOI: 10.1063/5.0094875
127. Hong Gong, Yao Wang*, **Xiao Zheng**, Rui-Xue Xu, and YiJing Yan*, “Nonequilibrium work distributions in quantum impurity system-bath mixing processes”, *J. Chem. Phys.* **157**, 054109 (2022). DOI: 10.1063/5.0095549
128. Qingfeng Zhuang, Lyuzhou Ye, and **Xiao Zheng***, “Competition between spin excitation and Kondo correlation in magnetic molecular junctions: Theoretical insight from first-principles-based simulations”, *Current Chinese Science* **2**, 310-324 (2022). DOI: 10.2174/2210298102666220302095638
129. Yun-An Yan*, **Xiao Zheng**, and Jiushu Shao, “Piecewise ensemble averaging stochastic Liouville equations for simulating non-Markovian quantum dynamics”, *New J. Phys.* **24**, 103012 (2022). DOI: 10.1088/1367-2630/ac94f1
130. Ya-Rong Zheng†, ShaoJin Hu†, Xiao-Long Zhang†, Huanxin Ju, Zhenbin Wang, Peng-Ju Tan, Rui Wu, Fei-Yue Gao, Taotao Zhuang, **Xiao Zheng**, Junfa Zhu, Min-

- Rui Gao*, and Shu-Hong Yu*, “Black phosphorous mediates surface charge redistribution of CoSe₂ for electrochemical H₂O₂ production in acidic electrolytes”, *Adv. Mater.* **34**, 2205414 (2022). DOI: 10.1002/adma.202205414
131. Xu Ding, Daochi Zhang, Lyuzhou Ye*, **Xiao Zheng***, and YiJing Yan, “On the practical truncation tier of fermionic hierarchical equations of motion”, *J. Chem. Phys.* **157**, (22), 224107 (2022). DOI: 10.1063/5.0130355
132. Jiaan Cao[†], Lyuzhou Ye^{†*}, Dawei He, **Xiao Zheng***, and Shaul Mukamel, “Magnet-free time-resolved magnetic circular dichroism with pulsed vector beams”, *J. Phys. Chem. Lett.* **13**, (48), 11300-11306 (2022). DOI: 10.1021/acs.jpcllett.2c03370
133. Lijun Zuo, Qingfeng Zhuang, Lyuzhou Ye*, YiJing Yan, and **Xiao Zheng***, “Unveiling the decisive factor for the sharp transition in the scanning tunneling spectroscopy of a single nickelocene molecule”, *J. Phys. Chem. Lett.* **13**, (48), 11262-11270 (2022). DOI: 10.1021/acs.jpcllett.2c03168
134. Daochi Zhang[†], Lijun Zuo[†], Lyuzhou Ye, Zi-Hao Chen, Yao Wang, Rui-Xue Xu, **Xiao Zheng***, and YiJing Yan, “Hierarchical equations of motion approach for accurate characterization of spin excitations in quantum impurity systems”, *J. Chem. Phys.* **158**, (1), 014106 (2023). DOI: 10.1063/5.0131739
135. Xiaoli Wang, Qingfeng Zhuang, Ping Wu, Leifang Liu, Fang Wang, Xiaolei Zhang, Xiangyang Li*, and **Xiao Zheng**, “Tweezer-like magnetic tip control of the local spin state in the FeOEP/Pb(111) adsorption system: a preliminary exploration based on first-principles calculations”, *Nanoscale* **15**, (5), 2369-2376 (2023). DOI: 10.1039/d2nr04379c
136. Jiaan Cao, Lyuzhou Ye, Rui-Xue Xu, **Xiao Zheng***, and YiJing Yan, “Recent advances in fermionic hierarchical equations of motion method for strongly correlated quantum impurity systems”, *JUSTC* **53**, (3), 0302 (2023). DOI: 10.52396/JUSTC-2022-0164
137. JingChun Wang, Yao Wang, Rui-Xue Xu, GuanHua Chen, and **Xiao Zheng***, “A semilocal machine-learning correction to density functional approximations”, *J. Chem. Phys.* **158**, (15), 154107 (2023). DOI: 10.1063/5.0148438

PROCEEDINGS AND BOOK CHAPTERS

138. Jiang Wu, Guanhua Chen*, Jingchun Wang, and **Xiao Zheng**, “Redesigning density functional theory with machine learning”, *Quantum Chemistry in the Age of Machine Learning*, Chapter **23**, edited by Pavlo O. Dral (Elsevier, 2023). DOI: 10.1016/B978-0-323-90049-2.00010-X
139. Lei Cui, Rulin Wang, 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).
140. 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).

141. **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).
142. 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. “Nanomagnets on surface: an open-system perspective”, *2023 International Symposium on Open Quantum System Dynamics*, Hangzhou, April 2023.
2. “WYSIWYG-style theoretical simulation of open quantum systems”, *Seminar on the Frontiers of Theoretical and Computational Chemistry*, Tianjin, April 2023.
3. “Low-temperature dissipative dynamics of strongly correlated quantum impurity systems”, *Pacificchem 2021: Modeling exciton and charge dynamics in molecules and clusters toward optoelectronic applications*, Honolulu, HI, USA (online), December 2021.
4. “Environmental quantum effects on the influence and control of molecular spin states”, *The 14th National Quantum Chemistry Conference of the Chinese Chemical Society, 3rd Branch: Quantum, Classical and Statistical Reaction Dynamics*, Shanghai, October 2021.
5. “Low-temperature dissipative dynamics of strongly correlated quantum impurity systems”, *2021 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry*, Qingdao, July 2021.
6. “Environmental quantum effects on the influence and control of molecular spin states”, *The 14th North China Regional Five Provinces and Cities Chemistry Academic Seminar - Chemistry Theory and Mechanism*, Zhangjiakou, July 2021.
7. “Low-temperature dissipative dynamics of strongly correlated quantum impurity systems”, *Workshop “Structure, Dynamics, Spectroscopy”*, Hangzhou, July 2021.
8. “Designing novel exchange-correlation functionals in density functional theory with machine-learning techniques”, *The 32nd Chinese Chemical Society Annual Meeting, 1st Branch: Frontiers in Physical Chemistry*, Zhuhai, April 2021.
9. “Quantum dissipative dynamics in low-temperature environments”, *The 32nd Chinese Chemical Society Annual Meeting, 24th Branch: Quantum and Classical Dynamics in Chemistry*, Zhuhai, April 2021.
10. “Nonequilibrium quantum dissipative dynamics in the low temperature and strong coupling regime”, *Workshop on Nonequilibrium Phenomena in Quantum Materials*, Beijing, April 2021.
11. “Environmental quantum effects on the influence and control of molecular spin states”, *The 2nd Youth Symposium on Chemical Theory and Mechanism*, Hefei, November 2020.
12. “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.

13. “Strong electron correlation from the perspective of open quantum systems”, *Workshop on New Methods for Strongly Correlated Electrons*, Qingdao, October 2019.
14. “Strongly correlated open electronic systems: Theories and applications”, *Inaugural Workshop at Qingdao Institute for Theoretical and Computational Sciences*, Qingdao, August 2019.
15. “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.
16. “Strongly correlated open electronic systems: Theories and applications”, *2019 Telluride Workshop on “Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy”*, Telluride, CO, USA, July 2019.
17. “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.
18. “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.
19. “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.
20. “Theoretical investigation on the control of local spin states in adsorbed magnetic molecules”, *2018 Spin Mini Workshop: Exotic magnetic phenomena*, Chengdu, June 2018.
21. “Recent Progress in HEOM and SEOM methods for fermionic open quantum systems”, *2018 Workshop on Hierarchical and Stochastic Schrödinger Equations*, Xiamen, May 2018.
22. “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.
23. “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.
24. “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.
25. “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.
26. “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.

27. "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.
28. "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.
29. "Control of quantum states in adsorbed single molecular magnets", *2016 Workshop on Computational and Statistical Mechanics in Complex Systems*, Shenzhen, China, Nov 2016.
30. "Accurate simulation of single molecular magnets adsorbed on metal surfaces", *Workshop for Chinese Young Physical Chemists*, Dalian, China, Nov 2016.
31. "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.
32. "Theoretical investigations on strong electron correlation effects in magnetic molecules adsorbed on material surfaces", *30th Chinese Chemical Society Annual Meeting*, Dalian, China, Jul 2016.
33. "Local temperatures of quantum impurity systems out of equilibrium", *7th Asia-Pacific Conference of Theoretical and Computational Chemistry*, Kaohsiung, Taiwan, Jan 2016.
34. "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.
35. "Local temperatures of open systems out of equilibrium", *2015 Workshop on Computational and Statistical Mechanics in Complex Systems*, Beijing, China, Oct 2015.
36. "Local temperatures of quantum impurity systems out of equilibrium", *Workshop on Nonequilibrium Processes in Small Systems 2015*, Guiyang, China, July 2015.
37. "First-principles simulation of real-time electronic dynamics on surfaces of materials", *Progress in Electromagnetics Research Symposium 2015*, Prague, Czech Republic, July 2015.
38. "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.
39. "Hierarchical equations of motion method for quantum transport and quantum control", *Workshop on Frontiers of Quantum Information*, Hangzhou, China, May 2015.
40. "A hierarchical dynamics approach to strongly correlated quantum impurity systems", *Workshop on Quantum Simulation*, Hong Kong, China, Dec 2014.
41. "First-principles method for electronic dynamics on surfaces of materials", *Workshop on Computational Materials and Computational Biology*, Hong Kong, China, Nov 2014.

42. "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.
43. "Improving the accuracy of density functional approximations", *2014 Workshop on Computational and Statistical Mechanics in Complex Systems*, Changchun, China, Sep 2014.
44. "A scaling correction approach to density functional approximations", *2nd Chinese Young Chemical Physicists Forum*, Guiyang, China, Aug 2014.
45. "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.
46. "Applications of a hierarchical dynamics approach to quantum dissipation and quantum control", *Workshop on Quantum Dissipation and Quantum Control*, Lanzhou, China, Apr 2014.
47. "TDDFT for open systems", *Hong Kong Spring School on Quantum Simulation Methods*, Hong Kong, China, Apr 2014.
48. "A hierarchical dynamics approach and its applications to strongly correlated electronic systems", *International Conference on Computational Modeling Methods and Applications*, Changchun, China, Sept 2013.
49. "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.
50. "First principles method for complex open quantum systems and its applications", *Workshop for Chinese Young Physical Chemists*, Hangzhou, China, Apr 2013.
51. "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.
52. "Quantum mechanical methods for open systems: Theories and applications", *Workshop on Computational Statistical Mechanics of Complex Systems 2012*, Hefei, China, Oct 2012.
53. "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.
54. "Quantum mechanical methods for open systems: Theories and applications", *1st Chinese Young Chemical Physicists Forum*, Guiyang, China, Jul 2012.
55. "Quantum Liouville-space approach to strongly correlated quantum impurity systems", *International Conference on Theoretical and High Performance Computational Chemistry 2012*, Nanjing, China, Jul 2012.
56. "Hierarchical equations of motion approach to strongly correlated quantum impurity systems", *Workshop on Quantum Information, Quantum Dissipation and Associated Physics 2012*, Chengdu, China, Jun 2012.
57. "Improving band gap prediction in density functional theory from molecules to solids", *28th Chinese Chemical Society Annual Meeting*, Chengdu, China, Apr 2012.

58. "Improving band gap prediction in density functional theory from molecules to solids", *243rd American Chemical Society National Meeting*, San Diego, CA, USA, Mar 2012.
59. "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.
60. "Hierarchical equations of motion method for strongly correlated systems", *Workshop on computational and statistical mechanics for complex systems*, Chengdu, China, Sep 2011.
61. "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.
62. "Improving band gap prediction by density functional theory: From atoms to solids", *240th American Chemical Society National Meeting*, Boston, MA, USA, Aug 2010.
63. "Exact real-time dynamics of electron transport in mesoscopic systems", *American Physical Society March Meeting 2009*, Pittsburgh, PA, USA, Mar 2009.
64. "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.
65. "A first-principles method for open electronic systems", *231st American Chemical Society National Meeting*, Atlanta, GA, USA, Mar 2006.
66. "A first-principles method for open electronic systems", *The Ninth National Quantum Chemistry Academic Conference*, Guilin, China, Oct 2005.
67. "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.
68. "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

69. "Precise theoretical simulation on the control of quantum states in molecules on surfaces", *"Supercomputing Lecture series" Episode 3: Computation in Molecular Science Research*, Computer Network Information Center of Chinese Academy of Sciences, November 2022.
70. "Theory and computation for open quantum systems", Xiamen University, Xiamen, October 2022.
71. "Open quantum systems: Theories and applications", Westlake Physics Colloquium, Westlake University, Hangzhou, September 2022.
72. "Open quantum systems: Development and applications of theoretical methods", Nanjing University, Nanjing, January 2022.

73. "Open electronic systems at ultralow temperatures: Theories and applications", Nanjing University, Nanjing, August 2020.
74. "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.
75. "Strong electron correlation from the perspective of open quantum systems", New York University Shanghai, Shanghai, Nov 2019.
76. "Precise control of local quantum states in adsorbed magnetic molecules: First-principles-based studies", Hangzhou Normal University, Hanzhou, Apr 2019.
77. "A scaling correction approach for improving density functional approximations", Beijing Normal University, Beijing, China, Jun 2015.
78. "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.
79. "Hierarchical dynamics approach to strongly correlated quantum impurity systems and electronic dynamics on surfaces", East China Normal University, Shanghai, China, Jan 2013.
80. "Introduction to quantum mechanics of open systems", *2012 Summer school for graduate students "Theoretical Chemistry"*, Guangzhou, China, Aug 2012.
81. "Hierarchical equations of motion approach to strongly correlated quantum impurity systems", Guizhou Normal College, Guiyang, China, Apr 2012.
82. "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.