

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 Cu₂O microcrystals toward lead ions: A rational design for the determination of lead ions”, *Small* **11**, (21), 2493-2498 (2015). DOI: 10.1002/sml.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).
 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).
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).
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).
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).
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 dissipaton-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**, 123001 (2021).
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**, 6398-6404 (2021).

-
113. 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.* (accepted on May 20, 2021). DOI:10.1063/1674-0068/cjcp2104077
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. 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
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* (accepted on Nov 30, 2021). DOI:10.1007/s12274-021-4030-7
119. Xiongzi Zeng, Wei Hu, **Xiao Zheng**, Jin Zhao, Zhenyu Li^{*}, and Jinlong Yang^{*}, “Computational characterization of nanosystems”, *Chin. J. Chem. Phys.* (accepted on Jan 19, 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**, 2094-2100 (2022). DOI:10.1021/acs.jpcclett.2c00228

所有论文统计

年份	第一作者	通讯作者	非第一也非通讯	总数
2004	2	0	0	2
2005	0	0	1	1
2006	0	0	2	2
2007	1	0	2	3
2008	2	1	2	5
2009	2	1	0	3
2010	2	0	1	3
2011	2	1	2	5
2012	2	1	2	5
2013	2	5	3	10
2014	1	3	1	5
2015	1	6	3	10
2016	0	7	3	10
2017	0	3	6	9
2018	1	5	5	11
2019	0	5	4	9
2020	0	6	4	10
2021	0	6	7	13
2022	0	2	4	6
总计	18	52	52	122
近五年	1	27	30	58