Qijing Zheng

Department of Physics
University of Science & Technology of China
96 Jinzhai Rd., Hefei, Anhui, China, 230026

zqj@ustc.edu.cn +86-15856902802
Github: QijingZheng Google Scholar staff.ustc.edu.cn/~zqj/

Author of **45** refereed publications

Total Citations: **1138**

H-index: **18**

PROFESSIONAL EXPERIENCE

Associate Professor

Department of Physics,
University of Science & Technology of China

Mar. 2022 – now Hefei, Anhui

Research Associate Professor

Department of Physics,
University of Science & Technology of China

Oct. 2018 – Mar. 2022 Hefei, Anhui

Postdoctoral Researcher

Hefei National Laboratory of Physical Sciences at the Microscale,
University of Science & Technology of China

Jun. 2016 – Sep. 2018 Hefei, Anhui

- Supervisor: **Prof. Jinlong Yang**

Visiting Scholar

University of the Basque Country - UPV/EHU

Jan. 2014 – Jan. 2015 Donostia-San Sebastian, Spain

- Advisor: **Prof. Angel Rubio**

EDUCATION

Ph.D. in Physics

University of Science & Technology of China

Sep. 2009 – Jun. 2016 Hefei, Anhui

- Dissertation: "Non-adiabatic Molecular Dynamics Study of Ultrafast Charge Separation in TMD Heterostructures"
- Supervisor: **Prof. Jin Zhao**

B.Sc. in Applied Physics

University of Science & Technology of China

Sep. 2005 – Jul. 2009 Hefei, Anhui

AWARDS

NULL
Still waiting to be awarded…

RESEARCH INTERESTS

My research focuses on first-principles calculations on electronic structure and excited carrier dynamics in different *condensed matter systems*, trying to understand the behavior of electrons in multiscale, including time, energy, real and momentum space.

For this purpose, I have taken part in the development of the following codes:

- Main developer of Hefei-NAMD [1]
  Hefei-NAMD is an *ab initio* non-adiabatic molecular dynamics program based on time-dependent density functional theory and surface hopping methods to investigate ultrafast dynamics of excited carriers and their coupling to other quasiparticles in real and momentum space, energy and time scale.
- Developer of VaspBandUnfolding [2]
  VaspBandUnfolding is a python library for processing VASP WAVECAR files. With it, one can obtain the real-space wavefunctions, perform band unfolding, calcuate the NAC etc.

[1] https://github.com/QijingZheng/Hefei-NAMD
[2] https://github.com/QijingZheng/VaspBandUnfolding

SKILLS

- Programming:
  Python Numpy Matplotlib Fortran Bash LaTeX
- DFT Codes
  VASP Quantum Espresso ASE Phonopy
- Others
  Vim Emacs Gimp

GRANTS

Principle Investigator:

- Proton-tunneling Coupled Ultrafast Charge Transfer on TiO_2 Surface
  NSFC, Grant No. **11704363** (¥ 220 000), Jan. 2018 – Dec. 2020
- Theoretical Investigation of Exciton Dynamics in 2D Transition Metal Dichalcogenides
  NSFC, Grant No. **12174363** (¥ 620 000), Jan. 2022 – Dec. 2025

Participant:

- Ultrafast Dynamics on TiO_2 Surface
  NSFC, Grant No. **11620101003** (¥ 3 174 000), Jan. 2017 – Dec. 2021

PUBLICATIONS

45 papers in total. # indicates first authors and * corresponding authors.

2022

[1] Chu, Weibin#; Tan, Shijing; **Zheng**, **Qijing**; Fang, Wei; Feng, Yexin; Prezhdo, Oleg V.; Wang, Bing; Li, Xinzheng* and Zhao, Jin*, "Ultrafast Charge Transfer Coupled to Quantum Proton Motion at Molecule/Metal Oxide Interface," *Science Advances*, vol. 8, no. 24, eabo2675, Jun. 2022.

[2] Tu, Youyou#; Chu, Weibin; Shi, Yongliang; Zhu, Wenguang; **Zheng**, **Qijing*** and Zhao, Jin*, "High Photoreactivity on a Reconstructed Anatase TiO_2(001) Surface Predicted by *Ab Initio* Nonadiabatic Molecular Dynamics," *Journal of Physical Chemistry Letters*, vol. 13, pp. 5766–5775, Jun. 2022.

[3] Zheng, Zhenfa#; **Zheng**, **Qijing*** and Zhao, Jin*, "Spin-orbit Coupling Induced Demagnetization in Ni: *Ab Initio* Nonadiabatic Molecular Dynamics Perspective," *Physical Review B*, vol. 105, p. 085 142, 8 Feb. 2022.

[4] Zhang, Lili#; Chu, Weibin; **Zheng**, **Qijing*** and Zhao, Jin*, "Effects of Oxygen Vacancies on the Photoexcited Carrier Lifetime in Rutile TiO_2," *Physical Chemistry Chemical Physics*, vol. 24, pp. 4743–4750, Jan. 2022.

2021

[1] Gao, Chang#; Zhang, Lili; **Zheng**, **Qijing*** and Zhao, Jin*, "Tuning the Lifetime of Photoexcited Small Polarons on Rutile TiO_2 Surface via Molecular Adsorption," *Journal of Physical Chemistry C*, vol. 125, no. 49, pp. 27 275–27 282, Dec. 2021.

[2] Dai, Yanan#; **Zheng**, **Qijing#**; Ziffer, Mark E; Rhodes, Daniel; Hone, James; Zhao, Jin* and Zhu, Xiaoyang*, "Ultrafast Ferroelectric Ordering on the Surface of a Topological Semimetal $MoTe_2$," *Nano Letters*, vol. 21, no. 23, pp. 9903–9908, Nov. 2021.

[3] Feng, Nan#; Tian, Yunzhe; Han, Jian; Zheng, Zhenfa; Wang, Aolei; **Zheng**, **Qijing**; Zhao, Jin; Bi, Ke* and Xu, Ben*, "Phonon–phonon Interaction Assisted Electron–hole Recombination in WSe_2/hBN van der Waals Heterostructure," *Journal of Applied Physics*, vol. 130, no. 20, p. 205 708, Nov. 2021.

[4] Liu, Jianyi#; Jiang, Xiang; Li, Xintong; Ma, Xiaochuan; Sun, Xia; **Zheng**, **Qijing**; Cui, Xuefeng*; Tan, Shijing; Zhao, Jin* and Wang, Bing*, "Time- and Momentum-resolved Image-potential States of 2H-MoS_2 Surface," *Physical Chemistry Chemical Physics*, vol. 23, no. 46, pp. 26 336–26 342, Nov. 2021.

[5] Ding, Yiran#; Zeng, Mengqi#; **Zheng**, **Qijing**; Zhang, Jiaqian; Xu, Ding; Chen, Weiyin; Wang, Chenyang; Chen, Shulin; Xie, Yingying; Ding, Yu; Zheng, Shuting; Zhao, Jin; Gao, Peng and Fu, Lei*, "Bidirectional and Reversible Tuning of the Interlayer Spacing of Two-dimensional Materials," *Nature Communications*, vol. 12, no. 1, p. 5886, Oct. 2021.

[6] Zheng, Zhenfa#; Jiang, Xiang; Chu, Weibin; Zhang, Lili; Guo, Hongli; Zhao, Chuanyu; Wang, Yanan; Wang, Aolei; **Zheng**, **Qijing*** and Zhao, Jin*, "Investigation of *ab initio* Nonadiabatic Molecular Dynamics of Excited Carriers in Condensed Matter Systems," *Acta Physica Sinica*, vol. 70, no. 17, p. 177 101, Sep. 2021.

[7] Zhou, Xiaoli[#]; Hao, He; Zhang, Ying-Jie; **Zheng**, **Qijing**; Tan, Shijing[*]; Zhao, Jin; Chen, Hai-Bo; Chen, Jie-Jie; Gu, Ying[*]; Yu, Han-Qing and Liu, Xian-Wei[*], "Patterning of Transition Metal Dichalcogenides Catalyzed by Surface Plasmons with Atomic Precision,"
Chem, vol. 7, no. 6, pp. 1626–1638, Jun. 2021.

[8] Guo, Hongli[#]; Chu, Weibin; Prezhdo, Oleg V; **Zheng**, **Qijing**[*] and Zhao, Jin, "Strong Modulation of Band Gap, Carrier Mobility and Lifetime in Two-Dimensional Black Phosphorene through Acoustic Phonon Excitation,"
Journal of Physical Chemistry Letters, vol. 12, no. 16, pp. 3960–3967, Apr. 2021.

[9] Jiang, Xiang[#]; **Zheng**, **Qijing**; Lan, Zhenggang; Saidi, Wissam A; Ren, Xinguo and Zhao, Jin[*], "Real-Time GW-BSE Investigations on Spin-Valley Exciton Dynamics in Monolayer Transition Metal Dichalcogenide,"
Science Advances, vol. 7, no. 10, eabf3759, Mar. 2021.

[10] Zhang, Lili[#]; Chu, Weibin; Zhao, Chuanyu; **Zheng**, **Qijing**[*]; Prezhdo, Oleg V and Zhao, Jin, "Dynamics of Photoexcited Small Polarons in Transition-Metal Oxides,"
Journal of Physical Chemistry Letters, vol. 12, no. 9, pp. 2191–2198, Feb. 2021.

2020

[1] Tan, Shijing[#]; Feng, Hao; **Zheng**, **Qijing**; Cui, Xuefeng; Zhao, Jin; Luo, Yi; Yang, Jinlong; Wang, Bing[*] and Hou, J. G.[*], "Interfacial Hydrogen-Bonding Dynamics in Surface-facilitated Dehydrogenation of Water on TiO_2(110),"
Journal of the American Chemical Society, vol. 142, no. 2, pp. 826–834, Dec. 2020.

[2] Chu, Weibin[#]; **Zheng**, **Qijing**; Akimov, Alexey V.[*]; Zhao, Jin[*]; Saidi, Wissam A.[*] and Prezhdo, Oleg V.[*], "Accurate Computation of Nonadiabatic Coupling With Projector Augmented-Wave Pseudopotentials,"
Journal of Physical Chemistry Letters, vol. 11, no. 23, pp. 10 073–10 080, Nov. 2020.

[3] Su, Jianfeng[#]; **Zheng**, **Qijing**; Shi, Yongliang[*] and Zhao, Jin[*], "Interlayer Polarization Explains Slow Charge Recombination in Two-Dimensional Halide Perovskites by Nonadiabatic Molecular Dynamics Simulation,"
Journal of Physical Chemistry Letters, vol. 11, no. 21, pp. 9032–9037, Oct. 2020.

[4] Fu, Cen Feng[#]; Zhao, Chuanyu; **Zheng**, **Qijing**; Li, Xingxing[*]; Zhao, Jin and Yang, Jinlong[*], "Halogen Modified Two-Dimensional Covalent Triazine Frameworks as Visible-light Driven Photocatalysts for Overall Water Splitting,"
Science China Chemistry, vol. 63, no. 8, pp. 1134–1141, Jun. 2020.

[5] Guo, Hongli[#]; Chu, Weibin; **Zheng**, **Qijing**[*] and Zhao, Jin[*], "Tuning the Carrier Lifetime in Black Phosphorene Through Family Atom Doping,"
Journal of Physical Chemistry Letters, vol. 11, no. 12, pp. 4662–4667, May 2020.

[6] Chu, Weibin[#]; **Zheng**, **Qijing**; Prezhdo, Oleg V.; Zhao, Jin[*] and Saidi, Wissam A.[*], "Low-Frequency Lattice Phonons in Halide Perovskites Explain High Defect Tolerance Toward Electron-Hole Recombination,"
Science Advances, vol. 6, no. 7, eaaw7453, Feb. 2020.

[7] Chu, Weibin[#]; **Zheng**, **Qijing**; Prezhdo, Oleg V. and Zhao, Jin[*], "CO_2 Photoreduction on Metal Oxide Surface Is Driven by Transient Capture of Hot Electrons: *Ab Initio* Quantum Dynamics Simulation,"
Journal of the American Chemical Society, vol. 142, no. 6, pp. 3214–3221, Jan. 2020.

[8] Tian, Yunzhe[#]; **Zheng**, **Qijing**[*] and Zhao, Jin[*], "Tensile Strain-Controlled Photogenerated Carrier Dynamics at the van der Waals Heterostructure Interface,"
Journal of Physical Chemistry Letters, vol. 11, no. 3, pp. 586–590, Jan. 2020.

2019

[1] Chen, Caiyun[#]; Kong, Longjuan[#]; Wang, Yu; Cheng, Peng; Feng, Baojie; **Zheng**, **Qijing**; Zhao, Jin[*]; Chen, Lan[*] and Wu, Kehui, "Dynamics of Single-Molecule Dissociation by Selective Excitation of Molecular Phonons,"
Physical Review Letters, vol. 123, no. 24, p. 246 804, Dec. 2019.

[2] Xie, Yu[#]; Sun, Huijuan; **Zheng**, **Qijing**; Zhao, Jin; Ren, Hao[*] and Lan, Zhenggang[*], "Diabatic Hamiltonian Construction in van der Waals Heterostructure Complexes,"
Journal of Materials Chemistry A, vol. 7, no. 48, pp. 27 484–27 492, Nov. 2019.

[3] Nie, Zhonghui[#]; Shi, Yongliang; Qin, Shuchao; Wang, Yuhan; Jiang, Hongzhu; **Zheng**, **Qijing**; Cui, Yang; Meng, Yuze; Song, Fengqi; Wang, Xiaoyong; Turcu, Ion C.E.; Wang, Xinran; Xu, Yongbing; Shi, Yi; Zhao, Jin[*]; Zhang, Rong[*] and Wang, Fengqiu[*], "Tailoring Exciton Dynamics of Monolayer Transition Metal Dichalcogenides by Interfacial Electron-Phonon Coupling,"
Communications Physics, vol. 2, no. 1, p. 103, Sep. 2019.

[4] Zhang, Lili[#]; Chu, Weibin; **Zheng**, **Qijing**; Benderskii, Alexander V.; Prezhdo, Oleg V.[*] and Zhao, Jin[*], "Suppression of Electron-Hole Recombination by Intrinsic Defects in 2D Monoelemental Material,"

Journal of Physical Chemistry Letters, vol. 10, no. 20, pp. 6151–6158, Sep. 2019.

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Physical Review B, vol. 99, no. 16, p. 165 309, Apr. 2019.

[7] **Zheng**, **Qijing**[#]; Chu, Weibin; Zhao, Chuanyu; Zhang, Lili; Guo, Hongli; Wang, Yanan; Jiang, Xiang and Zhao, Jin [*], "Ab Initio Nonadiabatic Molecular Dynamics Investigations on the Excited Carriers in Condensed Matter Systems,"
Wiley Interdisciplinary Reviews: Computational Molecular Science, vol. 9, no. 6, e1411, Mar. 2019.

[8] Niu, Xianghong[#]; Li, Yunhai; Zhang, Yehui; **Zheng**, **Qijing**; Zhao, Jin [*] and Wang, Jinlan [*], "Highly Efficient Photogenerated Electron Transfer at A Black Phosphorus/Indium Selenide Heterostructure Interface From Ultrafast Dynamics,"
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[9] Sun, Huijuan[#]; **Zheng**, **Qijing** [*]; Lu, Wencai and Zhao, Jin [*], "Ultrafast Dynamics of Solvated Electrons at Anatase TiO_2/H_2O Interface,"
Journal of Physics Condensed Matter, vol. 31, no. 11, p. 114 004, Jan. 2019.

2018

[1] Tan, Shijing[#]; Feng, Hao; Ji, Yongfei; **Zheng**, **Qijing**; Shi, Yongliang; Zhao, Jin; Zhao, Aidi; Yang, Jinlong; Luo, Yi; Wang, Bing [*] and Hou, J. G. [*], "Visualizing Elementary Reactions of Methanol by Electrons and Holes on TiO_2(110) Surface,"
Journal of Physical Chemistry C, vol. 122, no. 50, pp. 28 805–28 814, Nov. 2018.

[2] Zhang, Ruiqi[#]; Zhang, Lili[#]; **Zheng**, **Qijing**; Gao, Pengfei; Zhao, Jin [*] and Yang, Jinlong [*], "Direct Z-Scheme Water Splitting Photocatalyst Based on Two-dimensional van der Waals Heterostructures,"
Journal of Physical Chemistry Letters, vol. 9, no. 18, pp. 5419–5424, Sep. 2018.

[3] Guo, Hongli[#]; Zhao, Chuanyu; **Zheng**, **Qijing** [*]; Lan, Zhenggang; Prezhdo, Oleg V.; Saidi, Wissam A. and Zhao, Jin [*], "Superatom Molecular Orbital as An Interfacial Charge Separation State,"
Journal of Physical Chemistry Letters, vol. 9, no. 12, pp. 3485–3490, Jun. 2018.

[4] Wang, Yanan[#]; Guo, Hongli; **Zheng**, **Qijing** [*]; Saidi, Wissam A. and Zhao, Jin [*], "Tuning Solvated Electrons by Polar-Nonpolar Oxide Heterostructure,"
Journal of Physical Chemistry Letters, vol. 9, no. 11, pp. 3049–3056, Jun. 2018.

[5] **Zheng**, **Qijing**[#]; Xie, Yu; Lan, Zhenggang; Prezhdo, Oleg V.; Saidi, Wissam A. and Zhao, Jin [*], "Phonon-Coupled Ultrafast Interlayer Charge Oscillation at van der Waals Heterostructure Interfaces,"
Physical Review B, vol. 97, no. 20, p. 205 417, May 2018.

[6] Zhang, Lili[#]; **Zheng**, **Qijing**[#]; Xie, Yu; Lan, Zhenggang; Prezhdo, Oleg V.; Saidi, Wissam A. and Zhao, Jin [*], "Delocalized Impurity Phonon Induced Electron-Hole Recombination in Doped Semiconductors,"
Nano Letters, vol. 18, no. 3, pp. 1592–1599, Mar. 2018.

2017

[1] Zhao, Chuanyu[#]; **Zheng**, **Qijing** [*]; Wu, Jianlan and Zhao, Jin [*], "Ab Initio Nonadiabatic Molecular Dynamics Investigation on the Dynamics of Photogenerated Spin Hole Current in Cu-Doped MoS_2,"
Physical Review B, vol. 96, no. 13, p. 134 308, Oct. 2017.

[2] **Zheng**, **Qijing**[#]; Saidi, Wissam A.; Xie, Yu; Lan, Zhenggang; Prezhdo, Oleg V.; Petek, Hrvoje and Zhao, Jin [*], "Phonon-Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface,"
Nano Letters, vol. 17, no. 10, pp. 6435–6442, Oct. 2017.

2016

[1] Chu, Weibin[#]; Saidi, Wissam A.; **Zheng**, **Qijing** [*]; Xie, Yu; Lan, Zhenggang; Prezhdo, Oleg V.; Petek, Hrvoje and Zhao, Jin [*], "Ultrafast Dynamics of Photongenerated Holes at a CH_3OH/TiO_2 Rutile Interface,"
Journal of the American Chemical Society, vol. 138, no. 41, pp. 13 740–13 749, Oct. 2016.

[2] **Zheng**, **Qijing**[#]; Tan, Shijing[#]; Feng, Hao; Cui, Xuefeng [*]; Zhao, Jin and Wang, Bing [*], "Dynamic Equilibrium of Reversible Reactions and Migration of Hydrogen Atoms Mediated by Diffusive Methanol on Rutile TiO_2(110)-(1$\times$1) Surface,"

Journal of Physical Chemistry C, vol. 120, no. 14, pp. 7728–7735, Apr. 2016.

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Journal of Physical Chemistry C, vol. 120, no. 10, pp. 5503–5514, Feb. 2016.

2014

[1] Zhao, Jin[# *]; **Zheng**, **Qijing**; Petek, Hrvoje[*] and Yang, Jinlong[*], "Nonnuclear Nearly Free Electron Conduction Channels Induced by Doping Charge in Nanotube-Molecular Sheet Composites,"
Journal of Physical Chemistry A, vol. 118, no. 35, pp. 7255–7260, Sep. 2014.

2010

[1] He, Yu[#]; Wu, Tao; Wu, Gang; **Zheng**, **Qijing**; Liu, Yuzhe; Chen, Hong; Ying, Jianju; Liu, Ronghua; Wang, Xiangfeng; Xie, Yali; Yan, Yajun; Dong, J. K.; Li, Shiyang and Chen, Xianhui[*], "Evidence for Competing Magnetic and Superconducting Phases in Superconducting $Eu_{1-x}Sr_xFe_{2-y}Co_yAs_2$ Single Crystals,"
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Physical Review B, vol. 81, no. 5, p. 52 503, Feb. 2010.