

Qijing Zheng

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Author of **49** refereed publications

Total Citations: **1865**

H-index: **25**

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, calculate the NAC etc.

¹<https://github.com/QijingZheng/Hefei-NAMD>

²<https://github.com/QijingZheng/VaspBandUnfolding>

SKILLS

Programming:

Python Numpy Matplotlib Fortran
Bash L^AT_EX

DFT Codes

VASP Quantum Espresso ASE Phonopy

Others

Vim Emacs Gimp

GRANTS

Principle Investigator:

- Proton-tunneling Coupled Ultrafast Charge Transfer on TiO₂ 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 TiO₂ Surface
NSFC, Grant No. 11620101003 (¥ 3 174 000), Jan. 2017 – Dec. 2021

PUBLICATIONS

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

2023

- [1] Wang, Aolei[#]; Jiang, Xiang^{*}; Zheng, Qijing; Petek, Hrvoje and Zhao, Jin^{*}, "Ultrafast many-body bright-dark exciton transition in anatase tio₂," *Proc. Natl. Acad. Sci.*, vol. 120, no. 47, e2307671120, Nov. 2023.
- [2] Zheng, Zhenfa[#]; Shi, Yongliang^{*}; Zhou, Jin-Jian; Prezhdo, Oleg V.; Zheng, Qijing^{*} and Zhao, Jin^{*}, "Ab Initio Real-time Quantum Dynamics of Charge Carriers in Momentum Space," *Nature Computational Science*, vol. 3, pp. 352–541, Jun. 2023.
- [3] Tu, Youyou[#]; Zheng, Qijing^{*} and Zhao, Jin^{*}, "Research on Quantum Proton Coupled Charge Transfer Process Based on Deep Neural Network," *Frontiers of Data and Computing*, vol. 5, no. 2, pp. 37–49, Apr. 2023.

2022

- [1] Zhao, Chuanyu[#]; Zheng, Qijing and Zhao, Jin^{*}, "Excited Electron and Spin Dynamics in Topological Insulator: A Perspective from *ab initio* Non-adiabatic Molecular Dynamics," *Fundamental Research*, vol. 2, no. 4, pp. 506–510, Jul. 2022.
- [2] Chu, Weibin[#]; Tan, Shijing; Zheng, Qijing; Fang, Wei; Feng, Yexin; Prezhdo, Oleg V.; Wang, Bing; Li, Xinzhen^{*} 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.
- [3] Tu, Youyou[#]; Chu, Weibin; Shi, Yongliang; Zhu, Wenguang; Zheng, Qijing^{*} and Zhao, Jin^{*}, "High Photoreactivity on a Reconstructed Anatase TiO₂(001) Surface Predicted by *Ab Initio* Nonadiabatic Molecular Dynamics," *Journal of Physical Chemistry Letters*, vol. 13, pp. 5766–5775, Jun. 2022.
- [4] 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.
- [5] Zhang, Lili[#]; Chu, Weibin; Zheng, Qijing^{*} and Zhao, Jin^{*}, "Effects of Oxygen Vacancies on the Photoexcited Carrier Lifetime in Rutile TiO₂," *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 TiO₂ 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 MoTe₂," *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 WSe₂/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-MoS₂ 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.

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- [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 TiO₂(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.
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- [7] Chu, Weibin[#]; **Zheng, Qijing**; Prezhdo, Oleg V. and Zhao, Jin^{*}, “CO₂ 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.

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- [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.
- [5] Zheng, Zhenfa[#]; **Zheng, Qijing**^{*} and Zhao, Jin^{*}, "Ultrafast Electron Transfer Dynamics in Lateral Transition-Metal Dichalcogenide Heterostructures," *Electronic Structure*, vol. 1, no. 3, p. 034 001, Sep. 2019.
- [6] Wang, Yanan[#]; Shi, Yongliang; Zhao, Chuanyu; **Zheng, Qijing**^{*} and Zhao, Jin^{*}, "Photogenerated Carrier Dynamics at the Anatase/Rutile TiO₂ Interface," *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," *Journal of Materials Chemistry C*, vol. 7, no. 7, pp. 1864–1870, Jan. 2019.
- [9] Sun, Huijuan[#]; **Zheng, Qijing**^{*}; Lu, Wencai and Zhao, Jin^{*}, "Ultrafast Dynamics of Solvated Electrons at Anatase TiO₂/H₂O Interface," *Journal of Physics Condensed Matter*, vol. 31, no. 11, p. 114 004, Jan. 2019.

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- [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 TiO₂(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 MoS₂," *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 Photogenerated Holes at a CH₃OH/TiO₂ 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 TiO₂(110)-(1×1) Surface," *Journal of Physical Chemistry C*, vol. 120, no. 14, pp. 7728–7735, Apr. 2016.
- [3] Feng, Hao[#]; Tan, Shijing; Tang, Haoqi; Zheng, Qijing; Shi, Yongliang; Cui, Xuefeng^{*}; Shao, Xiang; Zhao, Aidi; Zhao, Jin and Wang, Bing^{*}, "Temperature- and Coverage-Dependent Kinetics of Photocatalytic Reaction of Methanol on TiO₂(110)-(1×1) Surface," *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.

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