Qijing Zheng

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Author of **46** 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

iii 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

a 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.

SKILLS

• Programming:

Python Numpy Matplotlib Fortran

Bash ETEX

DFT Codes

VASP Quantum Espresso ASE Phonopy

Others

Vim Emacs Gimp

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

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

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

- [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, 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.
- [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.

- [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. 26336–26342, 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.

- [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. 10073–10080, 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.
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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.

- [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. 27484–27492, 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.
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- [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.

- [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.
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- [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.

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- [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.

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- [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 CH₃OH/TiO₂ Rutile Interface," *Journal of the American Chemical Society*, vol. 138, no. 41, pp. 13740–13749, 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.

[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_yAs₂ Single Crystals," *Journal of Physics Condensed Matter*, vol. 22, no. 23, p. 235 701, May 2010.
- [2] Ying, Jianjun[#]; Wu, Tao; **Zheng**, **Qijing**; He, Yu; Wu, Gang; Li, Qiuju; Yan, Yajun; Xie, Yali; Liu, Ronghua; Wang, Xiangfeng and Chen, Xianhui *, "Electron Spin Resonance in EuFe_{1-x}Co_xAs₂ Single Crystals," *Physical Review B*, vol. 81, no. 5, p. 52 503, Feb. 2010.