Dr. Fujie Tang

Contact Information

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Academic positions

CSI Postdoctoral Scholar Oct. 2019 to Present
Joint Postdoc in Computational Chemical Science Center in Princeton University,
Temple University, Philadelphia, PA, U.S.A.
Supervisor: Prof. Xifan Wu

Postdoctoral Fellow Oct. 2018 to Sept. 2019
Department of Physics,
Temple University, Philadelphia, PA, U.S.A.
Supervisor: Prof. Xifan Wu

Education

Peking University, Beijing, P.R.China

Ph.D., Condensed Matter Physics Sept. 2013 to Jun. 2018

- Thesis Topic: *Structures and Dynamics of Interfacial Water*
- Supervisors: Prof. Limei Xu & Dr. Yuki Nagata

Peking University, Beijing, P.R.China

B.S., Major in Physics Sept. 2009 to Jul. 2013

Work Experience

Visiting Scholar Jun. 2019 to Jul. 2019
Department of Physics, University of California, Berkeley
Berkeley, CA, U.S.A.
Host: Prof. Steven G. Louie

Research Assistant Sept. 2013 to Jun. 2018
International Center for Quantum Materials,
Peking University, Beijing, P.R.China
Supervisor: Prof. Limei Xu

Visiting Student Jan. 2016 to Sept. 2016
Max Planck Institute for Polymer Research,
Mainz, Germany
Supervisors: Dr. Yuki Nagata & Prof. Dr. Mischa Bonn

Teaching Assistant Feb. 2015 to Jun. 2015
School of Physics, Peking University, Beijing, P.R.China

Awards and Honors

- Springer Thesis Award of 2018, Springer Nature Singapore. Aug. 2018
- The Excellent Doctoral Dissertation of Peking University. Jul. 2018
- Distinguished Graduate of Peking University. Jul. 2018
- National Scholarship for Doctoral Students, Ministry of Education, P.R.China.
  Top Honor for Graduate Student from Government. Oct. 2017
- Merit Students in Peking University. Peking University. Oct. 2017
- Special Scholarship for Doctoral Students. Peking University. Sept. 2016

- Selected by Everest Program, A National Program for Training Top Students in Fundamental Disciplines, Ministry of Education, P. R. China. Sept. 2010
- The 3rd Class Scholarship for Fresh Students, Peking University. Sept. 2009

Research Interests

- *Ab initio* calculation, GW/BSE calculation, *ab initio* molecular dynamics, classical molecular dynamics.
- Theory and simulation of sum frequency generation spectroscopy of interfacial structure, from gas phase/solid, gas phase/liquid interface, to liquid/solid. such as methanol/TiO_2, ice/air, ionic liquid/air, water/TiO_2, water/air, and ionic liquid/solid etc.
- X-ray absorption spectroscopy calculation for water, ice, and organic material; optical spectrum calculation of water.
- Structure and dynamics of ionic liquid; reconstruction and proton ordering of ice surface.
- Ferroelectric property and proton transferring behaviors in organic molecules.

Peer Reviewed Journals

Summary: 14 published papers (in reverse chronological order), 7 + 1(revising) first-author papers and total 481 citations (Google Scholar)

1. **Fujie Tang**, Jianhang Xu, Diana Y. Qiu and Xifan Wu. Impact of Nuclear Quantum Effects on the Electronic Structure of the Aqueous Solvation of the Chloride Ion. *Phys. Rev. B* Under review.
2. Chunyi Zhang, Linfeng Zhang, Jianhang Xu, **Fujie Tang**, Biswajit Santra, and Xifan Wu, Isotope Effects in X-ray Absorption Spectra of Liquid Water, *Phys. Rev. B*, 2020, **102**, 115155.
3. Hongwei Wang, **Fujie Tang**, Pratikkumar H. Dhuvad, and Xifan Wu, Interface Enhanced Functionalities in Oxide Superlattices under Mechanical and Electric Boundary Conditions, *npj Comput Mater*, 2020, **6**, 52.
4. **Fujie Tang**, Tatsuhiko Ohto, Shumei Sun, Jeremy R. Rouxel, Sho Imoto, Ellen H. G. Backus, Shaul Mukamel, Mischa Bonn, and Yuki Nagata. Molecular Structure and Modeling of Water-Air and Ice-Air Interfaces Monitored by Sum-frequency Generation. *Chem. Rev.*, 2020, **120**, 3633-3667.
5. **Fujie Tang**, Xuanyuan Jiang, Hsin-Yu Ko, Jianhang Xu, Mehmet Topsakal, Guanhua Hao, Alpha T. N'Diaye, Peter A. Dowben, Deyu Lu, Xiaoshan Xu, and Xifan Wu. Inversion Symmetry Breaking Probed by X-ray Absorption Spectroscopy in H-bonded Organic Ferroelectric Crystal. *Phys. Rev. Materials*, 2020, **4**, 034401.
6. Tatsuhiko Ohto, Mayank Dodia, Jianhang Xu, Sho Imoto, **Fujie Tang**, Frederik Zysk, Thomas D. Kuhne, Yasuteru Shigeta, Mischa Bonn, Xifan Wu, Yuki Nagata. Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Water–Air Interface. *J. Phys. Chem. Lett.*, 2019, **123**, 099602.
7. Ruidan Zhang, Jichao Dong, Ting Luo, **Fujie Tang**, Xingxing Peng, Chuanyao Zhou, Xueming Yang, Limei Xu, Zefeng Ren. Adsorption Structure and Coverage-Dependent Orientation Analysis of Submonolayer Acetonitrile on TiO_2(110). *J. Phys. Chem. C.*, 2019, **123**, 17915-17924.

8. Shumei Sun*, **Fujie Tang***, Sho Imoto, Daniel R Moberg, Tatsuhiko Ohto, Francesco Paesani, Mischa Bonn, and Yuki Nagata. Orientational Distribution of Free OH Groups of Interfacial Water is Exponential. *Phys. Rev. Lett.*, 2018. **121**, 246101. (*equal contribution)

9. Bart Weber, Yuki Nagata, Stephania Ketzetzi, **Fujie Tang**, Wilbert J. Smit, Huib J. Bakker, Ellen H.G. Backus, Mischa Bonn, and Daniel Bonn. Molecular Insight into the Slipperiness of Ice. *J. Phys. Chem. Lett.*, 2018, **9**, 2838.
Highlighted by Nature "Why your feet slip and slide on ice?"

10. **Fujie Tang**, Tatsuhiko Ohto, Taisuke Hasegawa, Wen Jun Xie, Limei Xu, Mischa Bonn, and Yuki Nagata. Definition of Free O-H Groups of Water at the Air-Water Interface. *J. Chem. Theory Comput.*, 2018, **14**, 357.

11. Wilbert J. Smit*, **Fujie Tang***, M. Alejandra Sanchez, Ellen H. G. Backus, Limei Xu, Taisuke Hasegawa, Mischa Bonn, Huib J. Bakker, and Yuki Nagata. Excess Hydrogen Bond at the Ice-Vapor Interface around 200 K. *Phys. Rev. Lett.*, 2017. **119**, 133003. (*equal contribution)

12. Wilbert J. Smit, **Fujie Tang**, Yuki Nagata, M. Alejandra Sanchez, Taisuke Hasegawa, Ellen H. G. Backus, Mischa Bonn, and Huib J. Bakker. Observation and Identification of a New OH Stretch Vibrational Band. *J. Phys. Chem. Lett.*, 2017, **8**, 3656.

13. Saman Hosseinpour*, **Fujie Tang***, Fenglong Wang, Ruth A. Livingstone, Simon J. Schlegel, Tatsuhiko Ohto, Mischa Bonn, Yuki Nagata, and Ellen H. G. Backus. Chemisorbed and Physisorbed Water at the TiO_2/Water Interface. *J. Phys. Chem. Lett.*, 2017, **8**, 2195. (*equal contribution)

14. **Fujie Tang**, Tatsuhiko Ohto, Taisuke Hasegawa, Mischa Bonn and Yuki Nagata. π^+–π^+ Stacking of Imidazolium Cations Enhances Molecular Layering of Room Temperature Ionic Liquids at Their Interfaces. *Phys. Chem. Chem. Phys.*, 2017, **19**, 2850.

15. Fivos Perakis, Luigi De Marco, Andrey Shalit, **Fujie Tang**, Zachary R. Kann, Thomas D. Kuhne, Renato Torre, Mischa Bonn, and Yuki Nagata. Vibrational Spectroscopy and Dynamics of Water. *Chem. Rev.*, 2016, **116**, 7590.

Books & Book Chapters

1. **Fujie Tang**. Structures and Dynamics of Interfacial Water: Input from Theoretical Vibrational Sum-frequency Spectroscopy. Springer Thesis Series 2019 (Recognizing Outstanding Ph.D. Research), ISBN 978-981-13-8964-1, by Springer Nature Singapore.

2. **Fujie Tang**, Takakazu Seki, Chun-Chieh Yu, Yuki Nagata. Microscopic Structure of Ice Surface Viewed through Sum-frequency Generation Spectroscopy. In a Chapter of "Chemistry of the Cryosphere", Advances in Atmospheric Chemistry, Vol. 3, by World Scientific Publishing. In Press.

3. **Fujie Tang**, Xifan Wu. Theoretical X-ray Absorption Spectroscopy of Liquid Water Using First Principles Calculations. In a Chapter of "Properties of Water from Numerical and Experimental Perspectives", by CRC Press. In Press.

Presentations

1. **Fujie Tang**. Seminar Talk. *Theoretical X-ray Absorption Spectroscopy of Liquid Water by the GW plus Bethe-Salpeter equation (GW-BSE) method.* Chemistry in Solution and at Interfaces (CSI) Center, Princeton University, Princeton, NJ, U.S.A. Online. Apr. 30, 2021

2. **Fujie Tang**. Oral Presentation. *Theoretical X-ray Absorption Spectroscopy of Liquid Water by the GW plus Bethe-Salpeter equation (GW-BSE) method.* American Physical Society, March Meeting, Online. Mar. 19, 2021

3. **Fujie Tang**. Seminar Talk. *Impact of Nuclear Quantum Effects on the Electronic Structure of Aqueous Solvation Chloride Ion.* In John P. Perdew's Group, Department of Physics, Temple University, PA, U.S.A. Jun. 17, 2020

4. **Fujie Tang**. Seminar Talk. *Molecular Modeling of Interfacial Water at Water-Air Interface and Ice-Air Interface.* Chemistry in Solution and at Interfaces (CSI) Center, Temple University, PA, U.S.A. Dec. 13, 2019

5. **Fujie Tang**. Invited Seminar Talk. *Molecular Modeling of Interfacial Water at Water-Air Interface and Ice-Air Interface.* In Arun Majumdar's Group, Department of Mechanical Engineering, Stanford University, CA, U.S.A. Jul. 19, 2019

6. **Fujie Tang**. Seminar Talk. *Molecular Modeling of Interfacial Water at Water-Air Interface and Ice-Air Interface.* In Steven G. Louie's Group, Department of Physics, University of California, Berkeley, CA, U.S.A. Jun. 27, 2019

7. **Fujie Tang**. Oral Presentation. *X-ray absorption spectroscopy signature of ferroelectricity in croconic acid.* American Physical Society, March Meeting, Boston, MA, U.S.A. Mar. 11-15, 2019

8. **Fujie Tang**. Oral Presentation. *Excess Hydrogen Bond at the Ice-Vapor Interface around 200K.* In the Forum of "PFUNT-Physics Five Universities The National Top" held in Peking University, Beijing, P.R.China. Dec. 15-17, 2017

9. **Fujie Tang**. Oral Presentation. *Definition of Free O-H Groups of Interfacial Water at Water-Air Interface.* In the Autumn Meeting for Chinese Physical Society held in Sichuan University, Chengdu, P.R.China. Sept. 8-11, 2017

10. **Fujie Tang**. Invited Talk. *Water Structure and Dynamics on Surfaces.* In the 11^{th} National Soft Matter Physics Conference held in Xiamen University, Xiamen, P.R.China. Mar. 24-27, 2017

11. **Fujie Tang**. Oral Presentation. *Analysis of Stress Sensitive Unstable Structures and Stability of a Metallic Glass by Simulated Nanoindentation.* In the 4^{th} Young Scientist Symposium of Soft Matter Physics held in Soochow University, Soochow, P.R.China. Oct. 16-17, 2015

Language and Software Skills

- Language: English(Fluent), Mandarin(Native).
- Computer Skills: C, C++, Fortran, Python, UNIX shell scripting, MATLAB, Mathematica.
- Softwares: CP2K, ORCA, LAMMPS, QUANTUM ESPRESSO, GROMACS and BerkeleyGW.

Journal Reviewer

Physical Review Letters, Physical Review B, Physical Review Materials, Journal of Physical Chemistry, Frontiers in Chemistry, International Journal of Quantum Chemistry, Journal of Colloid and Interface Science

Computer Allocations

Project PI Proxy FY2019, FY2020

- National Energy Research Scientific Computing Center (NERSC)
  PI: Prof. Xifan Wu

Teaching Experience	• Teaching Assistant for General Physics I	Feb. 2015 to Jun. 2015
Mentorship	• Jichao Dong (Grad from Peking University)	Jan. 2017 to Jul. 2018
	• Kefeng Shi (Grad from Temple University)	Aug. 2020 to Present

Professional Society Memberships: American Physics Society, American Chemical Society

References

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Max Planck Institute for Polymer Research, Mainz, Germany

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