Dr. Fujie Tang

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Academic positions

Postdoctoral Fellow — Oct. 2018 to Present
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 — Jun. 2018

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

Peking University, Beijing, P.R.China

B.S., Major in Physics — 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 and 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: 13 published papers (in reverse chronological order), 7 first-author papers and total 344 citations (Google Scholar)

1. Hongwei Wang, **Fujie Tang**, Pratikkumar H. Dhuvad, and Xifan Wu, Interface enhanced functionalities in oxide superlattices under mechanical and electric boundary conditions, *npj Computational Materials*, accepted.
2. **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.*, in press.
3. **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.
4. 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, **10**, 4914-4919.
5. 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.
6. 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)
7. 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.
8. **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.

9. 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)

10. 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.

11. 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)

12. **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.

13. 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 Chemistry of the cryosphere, Advances in Atmospheric Chemistry, by World Scientific. in press.

Presentations

1. **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

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

3. **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

4. **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

5. **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

6. **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

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

8. **Fujie Tang**. Oral Presentation. *Analysis of Stress Sensitive Unstable Structures and Stability of a Metallic Glass by Simulated Nanoindentation.* In the 4th 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.

References

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