

## Dr. Fujie Tang

---

CONTACT INFORMATION	Room 721, Science Education and Research Center Temple University Philadelphia, Pennsylvania 19122, U.S.A.	+1-302(521)6356 <a href="mailto:fujie.tang@temple.edu">fujie.tang@temple.edu</a> <a href="https://github.com/fujieku">fujieku.github.io</a>
ACADEMIC POSITIONS	<b>Postdoctoral Fellow</b> Department of Physics, Temple University, Philadelphia, PA, U.S.A. Supervisor: Prof. Xifan Wu	Oct. 2018 to Present
EDUCATION	<b>Peking University</b> , Beijing, P.R.China  Ph.D., Condensed Matter Physics • Thesis Topic: <i>Structures and Dynamics of Interfacial Water</i> • Advisor: Prof. Limei Xu & Dr. Yuki Nagata  <b>Peking University</b> , Beijing, P.R.China  B.S., Major in Physics	Jun. 2018       Jul. 2013
WORK EXPERIENCE	<b>Visiting Scholar</b> Department of Physics, University of California, Berkeley Berkeley, CA, U.S.A. Host: Prof. Steven G. Louie  <b>Research Assistant</b> International Center for Quantum Materials, Peking University, Beijing, P.R.China Supervisor: Prof. Limei Xu  <b>Visiting Student</b> Max Planck Institute for Polymer Research, Mainz, Germany Supervisors: Dr. Yuki Nagata and Prof. Dr. Mischa Bonn  <b>Teaching Assistant</b> School of Physics, Peking University, Beijing, P.R.China	Jun. 2019 to Jul. 2019           Sept. 2013 to Jun. 2018           Jan. 2016 to Sept. 2016       Feb. 2015 to Jun. 2015
AWARDS AND HONORS	<ul style="list-style-type: none"><li>• Springer Thesis Award of 2018, Springer Nature Singapore.</li><li>• The Excellent Doctoral Dissertation of Peking University.</li><li>• Distinguished Graduate of Peking University.</li><li>• National Scholarship for Doctoral Students, Ministry of Education, P.R.China Top Honor for Graduate Student from Government</li><li>• Merit Students in Peking University. Peking University.</li><li>• Special Scholarship for Doctoral Students. Peking University.</li><li>• Selected by Everest Program, A National Program for Training Top Students in Fundamental Disciplines, Ministry of Education, P. R. China.</li><li>• The 3<sup>rd</sup> Class Scholarship for Fresh Students, Peking University.</li></ul>	Aug. 2018 Jul. 2018 Jul. 2018 Oct. 2017 Oct. 2017 Sept. 2016 Sept. 2010 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<sub>2</sub>, ice/air, ionic liquid/air, water/TiO<sub>2</sub>, 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 350 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 Comput Mater*, **6**, 52 (2020).
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.*, 2020, **120**, 3633-3667.
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<sub>2</sub>(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<sub>2</sub>/Water Interface. *J. Phys. Chem. Lett.*, 2017, **8**, 2195. (\*equal contribution)
12. **Fujie Tang**, Tatsuhiko Ohto, Taisuke Hasegawa, Mischa Bonn and Yuki Nagata.  $\pi^+-\pi^+$  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 11<sup>th</sup> 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 4<sup>th</sup> 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, Journal of Physical Chemistry.

PROFESSIONAL  
SOCIETY  
MEMBERSHIPS

American Physics Society

REFERENCES

Prof. Limei Xu  
Professor, Deputy Director  
International Center for Quantum Materials  
Peking University, Beijing, P.R.China  
Phone: +86-10-62755043  
E-mail: limei.xu@pku.edu.cn

Dr. Yuki Nagata  
Group Leader  
The Molecular Spectroscopy Department  
Max Planck Institute for Polymer Research, Mainz, Germany  
Phone: +49-6131-379-380  
E-mail: nagata@mpip-mainz.mpg.de

Prof. Xifan Wu  
Associate Professor  
Department of Physics  
Temple University, Philadelphia, PA, USA  
Phone: +1-215-204-7627  
E-mail: xifanwu@temple.edu

Prof. Dr. Mischa Bonn  
Director  
The Molecular Spectroscopy Department  
Max Planck Institute for Polymer Research, Mainz, Germany  
Phone: +49-6131-379-161  
E-mail: bonn@mpip-mainz.mpg.de