

## Dr. Fujie Tang

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ACADEMIC POSITIONS	<b>CSI Postdoctoral Scholar</b> Joint Postdoc in Computational Chemical Science Center in Princeton University, Temple University, Philadelphia, PA, U.S.A. Supervisor: Prof. Xifan Wu	Oct. 2019 to Present
	<b>Postdoctoral Fellow</b> Department of Physics, Temple University, Philadelphia, PA, U.S.A. Supervisor: Prof. Xifan Wu	Oct. 2018 to Sept. 2019
EDUCATION	<b>Peking University</b> , Beijing, P.R.China  Ph.D., Condensed Matter Physics • Thesis Topic: <i>Structures and Dynamics of Interfacial Water</i> • Supervisors: Prof. Limei Xu & Dr. Yuki Nagata	Sept. 2013 to Jun. 2018
	<b>Peking University</b> , Beijing, P.R.China  B.S., Major in Physics	Sept. 2009 to 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	Jun. 2019 to Jul. 2019
	<b>Research Assistant</b> International Center for Quantum Materials, Peking University, Beijing, P.R.China Supervisor: Prof. Limei Xu	Sept. 2013 to Jun. 2018
	<b>Visiting Student</b> Max Planck Institute for Polymer Research, Mainz, Germany Supervisors: Dr. Yuki Nagata & Prof. Dr. Mischa Bonn	Jan. 2016 to Sept. 2016
	<b>Teaching Assistant</b> School of Physics, Peking University, Beijing, P.R.China	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></ul>	Aug. 2018 Jul. 2018 Jul. 2018 Oct. 2017 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 3<sup>rd</sup> Class Scholarship for Fresh Students, Peking University. Sept. 2009

#### RESEARCH INTERESTS

- Electronic structure theory, GW/BSE excited states calculation, molecular dynamics simulation, machine learning applications in the molecular dynamic simulation.
- Theory and simulation of sum frequency generation spectroscopy of interfacial structure: water/air interface, ice, solid/water interfaces, etc.
- X-ray absorption spectroscopy calculation of water, ice, and organic material; Optical spectroscopy calculation of water.
- Theoretical modeling of the structure and dynamics of the ionic liquid;
- Reconstruction and proton ordering of the ice surface.
- Theoretical modeling of the ions in the aqueous solution: electronic structure and nuclear quantum effects.
- Ferroelectric property and proton transferring behaviors in organic molecules.

#### PEER REVIEWED JOURNALS

**Highlights:** 15 published papers, first/co-first author papers = 8, cited 508 times, h-index = 10.

Google Scholar: <https://scholar.google.com/citations?user=-Rx1hiIAAAAJ&hl=en>

1. **Fujie Tang**, Zhenglu Li, Chunyi Zhang, Steven G. Louie, Roberto Car, Diana Y. Qiu and Xifan Wu. Theoretical X-ray Absorption Spectroscopy of Liquid Water by the GW plus Bethe-Salpeter equation (GW-BSE) method. In preparation.
2. Chunyi Zhang, **Fujie Tang**, Mohan Chen, Linfeng Zhang, Diana Y. Qiu, John P. Perdew, Michael L. Klein, Xifan Wu. Modeling liquid water by climbing up Jacob's ladder in density functional theory facilitated by using deep neural network potentials. *J. Phys. Chem. B* Under review.
3. **Fujie Tang**, Jianhang Xu, Diana Y. Qiu and Xifan Wu. Nuclear quantum effects on the quasiparticle properties of the chloride anion aqueous solution within the GW approximation. *Phys. Rev. B*, 2021, **104**, 035117.
4. 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.
5. 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.
6. **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.
7. **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.
8. 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.
  9. 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.
  10. 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)
  11. 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?”
  12. **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.
  13. 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)
  14. 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.
  15. 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)
  16. **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.
  17. 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**. Invited Seminar Talk. *Theoretical X-ray Absorption Spectroscopy of Liquid Water by the GW plus Bethe-Salpeter equation (GW-BSE) method*. The Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPPEM), Department of Physics, University of California at Berkeley, Berkeley, CA, U.S.A. Online. Jul. 20, 2021
2. **Fujie Tang**. Seminar Talk. *Theoretical X-ray Absorption Spectroscopy of Liquid Water by the GW plus Bethe-Salpeter equation (GW-BSE) method*. The Chemistry in Solution and at Interfaces (CSI) Center, Princeton University, Princeton, NJ, U.S.A. Online. Apr. 30, 2021
3. **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
4. **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
5. **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
6. **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
7. **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
8. **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
9. **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
10. **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
11. **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
12. **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	<ul style="list-style-type: none"> <li>• Language: English(Fluent), Mandarin(Native).</li> <li>• Computer Skills: C, C++, Fortran, Python, UNIX shell scripting, MATLAB, Mathematica.</li> <li>• Softwares: CP2K, ORCA, LAMMPS, DeePMD-kit, QUANTUM ESPRESSO, GROMACS and BerkeleyGW.</li> </ul>	
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	<b>Project PI Proxy</b> <ul style="list-style-type: none"> <li>• National Energy Research Scientific Computing Center (NERSC) PI: Prof. Xifan Wu</li> </ul>	FY2019, FY2020, FY2021
TEACHING EXPERIENCE	<ul style="list-style-type: none"> <li>• Teaching Assistant for General Physics I</li> </ul>	Feb. 2015 to Jun. 2015
MENTORSHIP	<ul style="list-style-type: none"> <li>• Jichao Dong (Grad from Peking University)</li> <li>• Kefeng Shi (Grad from Temple University)</li> </ul>	Jan. 2017 to Jul. 2018 Aug. 2020 to Present
PROFESSIONAL SOCIETY MEMBERSHIPS	American Physics Society, American Chemical Society	
REFERENCES	<p>Prof. Limei Xu  Professor  International Center for Quantum Materials  Peking University, Beijing, P.R.China</p> <p>Dr. Yuki Nagata  Group Leader  The Molecular Spectroscopy Department  Max Planck Institute for Polymer Research, Mainz, Germany</p> <p>Prof. Xifan Wu  Professor  Department of Physics  Temple University, Philadelphia, PA, U.S.A.</p> <p>Prof. Mischa Bonn  Director  The Molecular Spectroscopy Department  Max Planck Institute for Polymer Research, Mainz, Germany</p>	
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