

## Fujie Tang (汤富杰), Ph.D.

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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  <b>Postdoctoral Fellow</b> Department of Physics, Temple University, Philadelphia, PA, U. S. A. Supervisor: Prof. Xifan Wu	2019.10-present  2018.10-2019.09
EDUCATION	<b>Peking University</b> , Beijing, P. R. China  Ph.D., Condensed Matter Physics • Thesis Topic: <i>Structures and Dynamics of Interfacial Water</i> • Supervisor: Prof. Limei Xu  <b>Max Planck Institute for Polymer Research</b> , Mainz, Germany  Visiting Ph.D. Student • Supervisors: Dr. Yuki Nagata & Prof. Mischa Bonn  <b>Peking University</b> , Beijing, P. R. China  B.S., Major in Physics	2013.09-2018.06  2016.01-2016.10  2009.09-2013.07
RESEARCH INTERESTS	1. First-principles calculations in the condensed phase materials, algorithms and applications: • electronic structure level: density functional theory, quantum chemistry, GW-BSE excited states calculations; • atomic/molecular structure and dynamic level: <i>ab initio</i> molecular dynamics simulation, path-integral molecular dynamics simulation, deep potential molecular dynamics simulation; 2. Advanced computational spectroscopic methods in the condensed phase materials, algorithms and applications: • Sum-frequency generation (SFG) spectroscopy, X-ray absorption (XAS) spectroscopy, optical spectroscopy, photoemission spectroscopy, etc.;	

3. Accurate modeling of the condensed phase systems, such as: liquid water/ice, solid surface, solid/liquid interface, confined system, low-dimensional material surface, aqueous solution, ionic liquid, amorphous/disorder systems, chemical reactions, etc.;

## RESEARCH

## EXPERIENCE

**CSI Postdoctoral Scholar:** Temple University 2019.10-present

Work with Prof. Xifan Wu, Prof. Michael L. Klein & Prof. Roberto Car

- Developed a novel GW-BSE workflow to calculate XAS spectra of liquid water from *ab initio*, revealed many-body effects beyond conventional BSE calculations;
- Simulated the impact of nuclear quantum effects on the photoemission spectra of  $\text{Cl}^-$  anion aqueous solutions;
- Studied the optical spectra of liquid water and ice by using GW-BSE method, established the connections between spectral feature and its molecular origins;
- Applied machine learning approach to stabilize the OH radical structure in solution, and computed the redox/oxidized potential of  $\text{OH}/\text{OH}^-$ ;

**Visiting Scholar:** University of California at Berkeley 2019.06-2019.07

Host: Prof. Steven G. Louie

- Initiated the XAS calculation by using GW-BSE method with BerkeleGW package;

**Postdoctoral Fellow:** Temple University 2018.10-2019.09

Work with Prof. Xifan Wu

- Proposed a method to probe the ferroelectricity in a molecular crystal by using XAS spectroscopy, validated by experiment;

**Research Assistant:** Peking University 2013.09-2018.06

Work with Prof. Limei Xu, Dr. Yuki Nagata, and Prof. Mischa Bonn

- Developed a new free-OH definition to investigate the water/air interface, found the exponential decay orientational behaviors of the free-OH groups, confirmed by experiment;
- Applied classical molecular dynamics simulation and theoretical SFG calculation to investigate the ice/air interface, found excess H-bond phenomenon at ice surface and a new vibrational band of ice SFG spectra, confirmed by experiment;
- Proposed a microscopic mechanism to explain the slipperiness of ice, with the combination of molecular dynamics simulation, theoretical SFG calculation and experimental measurement;

**Visiting Student:** Max Planck Institute for Polymer Research 2016.01-2016.10

Work with Dr. Yuki Nagata & Prof. Mischa Bonn

- Applied *ab initio* molecular dynamics simulation and theoretical SFG calculation to investigate the  $\text{TiO}_2$ /water interfaces, found chemisorbed and physisorbed water molecules at surface, confirmed by experiment;
- Investigate the ionic liquid by using *ab initio* molecular dynamics simulation, found its interface stabilized by  $\pi^+-\pi^+$  stacking interaction of imidazolium cations;

AWARDS AND  
HONORS

- Springer Thesis Award of 2018, Springer Nature Singapore. 2018.08
- The Excellent Doctoral Dissertation of Peking University. 2018.07
- Distinguished Graduate of Peking University. 2018.07
- National Scholarship for Doctoral Students, Ministry of Education, P. R. China.  
Top Honor for Graduate Student from Government. 2017.10
- Merit Students in Peking University. Peking University. 2017.10
- Special Scholarship for Doctoral Students. Peking University. 2016.09
- Selected by Everest Program, A National Program for Training Top Students  
in Fundamental Disciplines, Ministry of Education, P. R. China. 2010.09
- The 3<sup>rd</sup> Class Scholarship for Fresh Students, Peking University. 2009.09

PEER REVIEWED  
JOURNALS

**Highlights:** 19 published papers, first/co-first author papers = 9, cited 718 times, h-index = 11. (Updated: 07-08-2022)

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

1. Chun-Chieh Yu, Takakazu Seki, Kuo-Yang Chiang, **Fujie Tang**, Shumei Sun, Mischa Bonn and Yuki Nagata. Polarization-Dependent Heterodyne-Detected Sum Frequency Generation Spectroscopy as a Tool to Explore Surface Molecular Orientation and Ångströmscale Depth Profiling. *J. Phys. Chem. B*, accepted.
2. **Fujie Tang**, Zhenglu Li, Chunyi Zhang, Steven G. Louie, Roberto Car, Diana Y. Qiu and Xifan Wu. Many-body Effects in the X-ray Absorption Spectra of Liquid Water. *Proc. Natl. Acad. Sci. U.S.A.*, 2022, **119**, e2201258119.
3. Hongwei Wang, **Fujie Tang**, Massimiliano Stengel, Hongjun Xiang, Qi An, Tony Low, and Xifan Wu. Convert Widespread Paraelectric Perovskite to Ferroelectrics. *Phys. Rev. Lett.*, 2022, **128**, 197601.
4. 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*, 2021, 125, 11444-11456.  
**Selected as a Cover Art Article.**
5. **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.
6. 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.

7. 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.
8. **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.
9. **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. Probing Ferroelectricity by X-ray Absorption Spectroscopy in Molecular Crystals. *Phys. Rev. Materials*, 2020, **4**, 034401.
10. 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.
11. 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.
12. 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)
13. 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?”**
14. **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.
15. 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)
16. 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.

17. 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)
18. **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.
19. 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. Chapter 3 of “Chemistry of the Cryosphere”, Advances in Atmospheric Chemistry, Vol. 3, pp. 139-171 (2021), by World Scientific Publishing.
3. **Fujie Tang**, Xifan Wu. Theoretical X-ray Absorption Spectroscopy of Liquid Water Using First Principles Calculations. Chapter 1 of “Properties of Water from Numerical and Experimental Perspectives”, by CRC Press. In Press.

#### PRESENTATIONS AND POSTERS

1. **Fujie Tang**. Poster. International Workshop on Recent Developments in Electronic Structure (ES22), Columbia University, New York City, NY, U. S. A. 2022.06
2. **Fujie Tang**. Oral Presentation (virtual). American Physical Society, March Meeting. 2022.03
3. **Fujie Tang**. Seminar Talk (virtual). The Chemistry in Solution and at Interfaces (CSI) Center, Princeton University, Princeton, NJ, U. S. A. 2022.01
4. **Fujie Tang**. Invited Seminar Talk (virtual). Department of Physics, University of California at Berkeley, Berkeley, CA, U. S. A. 2021.07
5. **Fujie Tang**. Seminar Talk (virtual). Department of Physics, Temple University, Philadelphia, PA, U. S. A. 2021.07
6. **Fujie Tang**. Seminar Talk (virtual). The Chemistry in Solution and at Interfaces (CSI) Center, Princeton University, Princeton, NJ, U. S. A. 2021.04
7. **Fujie Tang**. Oral Presentation (virtual). American Physical Society, March Meeting. 2021.03

8. **Fujie Tang**. Seminar Talk. Department of Physics, Temple University, Philadelphia, PA, U. S. A. 2020.06
9. **Fujie Tang**. Seminar Talk. The Chemistry in Solution and at Interfaces (CSI) Center, Temple University, Philadelphia, PA, U. S. A. 2019.12
10. **Fujie Tang**. Invited Seminar Talk. Department of Mechanical Engineering, Stanford University, Stanford, CA, U.S.A. 2019.07
11. **Fujie Tang**. Seminar Talk. Department of Physics, University of California at Berkeley, Berkeley, CA, U. S. A. 2019.06
12. **Fujie Tang**. Oral Presentation. American Physical Society, March Meeting, Boston, MA, U. S. A. 2019.03
13. **Fujie Tang**. Oral Presentation. The Forum of "PFUNT-Physics Five Universities The National Top", Peking University, Beijing, P. R. China. 2017.12
14. **Fujie Tang**. Oral Presentation. The Autumn Meeting for Chinese Physical Society, Sichuan University, Chengdu, P. R. China. 2017.09
15. **Fujie Tang**. Invited Talk. The 11<sup>th</sup> National Soft Matter Physics Conference, Xiamen University, Xiamen, P. R. China. 2017.03
16. **Fujie Tang**. Oral Presentation. The 4<sup>th</sup> Young Scientist Symposium of Soft Matter Physics, Soochow University, Soochow, P. R. China. 2015.10

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, DeePMD-kit, LAMMPS, ORCA, QUANTUM ESPRESSO, GROMACS and BerkeleyGW.</li> </ul>
JOURNAL REVIEWER	Physical Review Letters, Physical Review A, 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> FY2019, FY2020, FY2021, FY2022 <ul style="list-style-type: none"> <li>• National Energy Research Scientific Computing Center (NERSC)</li> <li>PI: Prof. Xifan Wu</li> </ul>
TEACHING EXPERIENCE	<ul style="list-style-type: none"> <li>• Teaching Assistant for General Physics I Feb. 2015 to Jun. 2015</li> </ul>

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
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PROFESSIONAL SOCIETY MEMBERSHIPS	American Physics Society, American Chemical Society
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REFERENCES	<p>Prof. Limei Xu</p> <p>Professor</p> <p>International Center for Quantum Materials</p> <p>Peking University, Beijing, P. R. China</p> <p>Phone: +86-10-62755043</p> <p>E-mail: <a href="mailto:limei.xu@pku.edu.cn">limei.xu@pku.edu.cn</a></p> <p>Dr. Yuki Nagata</p> <p>Group Leader</p> <p>The Molecular Spectroscopy Department</p> <p>Max Planck Institute for Polymer Research, Mainz, Germany</p> <p>Phone: +49-6131-379-380</p> <p>E-mail: <a href="mailto:nagata@mpip-mainz.mpg.de">nagata@mpip-mainz.mpg.de</a></p> <p>Prof. Xifan Wu</p> <p>Professor</p> <p>Department of Physics</p> <p>Temple University, Philadelphia, PA, U. S. A.</p> <p>Phone: +1-215-204-7627</p> <p>E-mail: <a href="mailto:xifanwu@temple.edu">xifanwu@temple.edu</a></p> <p>Prof. Diana Y. Qiu</p> <p>Assistant Professor</p> <p>Department of Mechanical Engineering and Materials Science</p> <p>Yale University, New Haven, CT, U. S. A.</p> <p>Phone: +1-719-210-6447</p> <p>E-mail: <a href="mailto:diana.qiu@yale.edu">diana.qiu@yale.edu</a></p> <p>Prof. Mischa Bonn</p> <p>Director</p> <p>The Molecular Spectroscopy Department</p> <p>Max Planck Institute for Polymer Research, Mainz, Germany</p> <p>Phone: +49-6131-379-161</p> <p>E-mail: <a href="mailto:bonn@mpip-mainz.mpg.de">bonn@mpip-mainz.mpg.de</a></p>
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