Tian Tian

Assistant Profesor

Department of Chemical and Materials Engineering, University of Alberta

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Research Interests

- Machine learning for materials simulation and discovery
- Multiscale modeling of interfacial phenomena
- *Ab initio* electronic structure methods and high-throughput screening
- Software development and open-source tools for chemical and materials engineering

Academic Positions

2025 - now **University of Alberta, Canada**
Assistant Professor (Tenure-Track)

2025 - now **Alberta Machine Intelligence Institute (Amii), Canada**
Fellow

Education

Oct. 2015 - Mar. 2020 **ETH Zürich**
PhD, Chemical Engineering

Aug. 2012 - Jul. 2015 **Tsinghua University**
M.S., Chemistry

Aug. 2008 - Jul. 2012 **Tsinghua University**
B.S., Chemical Biology; Minor, Computer Technology and Application

Research Experience

Mar. 2023 - Dec. 2023 **Georgia Institute of Technology**
Postdoctoral Research (Supervisor: Prof. Andrew J. Medford & Prof. Phanish Suryanarayana)

- ML-powered computational workflow and toolkit for the `SPARC` quantum chemistry code
- Major developer for the `SPARC-X-API` simulation package

Dec. 2020 - Feb. 2023 **Carnegie Mellon University**
Postdoctoral Research (Supervisor: Prof. Zachary Ulissi)

- Machine learning methods for accelerating catalysis discovery
- Efficient catalyst computation workflow automation
- Transfer learning graph neural network models for computationally limited data regime

Apr. 2020 - Nov. 2020 **ETH Zürich**
Postdoctoral Research (Supervisor: Prof. Chih-Jen Shih)

- Theoretical analyses of interfacial dispersion forces affecting freestanding graphene.
- Experimental affirmation of repulsive van der Waals forces.

Oct. 2015 - Mar. 2020 **ETH Zürich**
Doctoral Projects (Supervisor: Prof. Chih-Jen Shih)

- Multiscale modeling of 2D materials interfaces
- Theoretical study of macroscopic phenomena on 2D materials
- Molecular epitaxy on 2D materials interfaces
- 2D material-based functional devices

Jun. 2017 - Sep. 2017 **Queen's University Belfast**
Research Internship (Supervisor: Prof. Elton G. J. Santos)

- *Ab initio* study of the dielectric nature of 2D materials
- Electric screening in 2D van der Waals heterostructures

Aug. 2012 - Jul. 2015 **Tsinghua University**
Master Thesis (Supervisor: Prof. Guangtao Li)

- Responsive polymer photonic crystal and for acetylcholinesterase assay
- Chemical and structural design in colloidal crystal microfluidic spheres using etching-reaction strategy
- Multi-functional patterned photonic crystal by alternative photolysis-reaction strategy

Jul. 2012 - Aug. 2012 **WWU Münster**
Research Internship (Supervisor: Prof. Bart Jan Ravoo)

- Synthesis of host-guest complex with tri-responsiveness for cyclodextrin vesicle linking

Nov. 2011 - Jul. 2012 **Tsinghua University**
Bachelor Thesis (Supervisor: Prof. Guangtao Li)

- Supramolecular assembly of main-chain bile acid polymers via copper-free click chemistry

Research Funding & Fellowships

2026 - NSERC Discovery Grant (applied)

2025 - 2027 UofA Startup funds
CAD 110,000

2021 - 2023 SNSF Early Postdoc Mobility Fellowship
CHF 115,550

Mentoring Experience

University of Alberta

2025 - now — Prince Ezeano (MSc Student)
ML for corrosion prediction; Theoretical simulation of high entropy alloy and oxide transformation (Collaboration: Prof. Jing Liu, UofA)

2025 - now — Mohammad Aarooj Yashin Ali (Research Assistant)
ML-acceleration of *ab initio* metadynamic simulations (Collaboration: Prof. Vinay Prasad, UofA)

Prior Mentoring Experience

2020 - 2025 — Gianluca Vagli (ETH Zürich, PhD Student)
Repulsive vdW simulation on 2D materials; AFM and metal nucleation experiments on suspended graphene (co-supervised with Prof. Chih-Jen Shih).
Outcomes: *Nat. Commun.* 2025, 16, 7726
Current position: Postdoc, ETH Zürich, Switzerland

2023 - 2024 — Lucas R Timmerman (GaTech, PhD Student)
Case testing for socket driver in SPARC-X-API project (mentored).
Outcomes: *J. Open Source Softw.* 2025, 10, 7747
Current position: PhD student, GaTech, USA

2021 - 2023 — Janghoon Ock (CMU, PhD Student)
Error cancellation of GNN models; catalyst energy simulation with BEEF-vdW functional (mentored)
Outcomes: *J. Chem. Phys.* 2023, 158, 214702
Current position: Assistant Professor, University of Nebraska Lincoln, USA

2021 - 2022 — Joe Musielewicz (CMU, PhD Student)
Integration of high-throughput VASP driver in FINETUNA project (mentored)
Outcomes: *Mach. Learn.: Sci. Technol.* 2022, 3, 03LT01
Current position: ML Scientist, Entalpic, USA

2022 - 2023 — Hilda Mera (CMU, PhD Student)
High-throughput computation using FINETUNA framework (mentored)
Current position: PhD student, CMU, USA

2018 - 2019 — Franzisca Naef (ETH Zürich, MSc Student)
Developing of Lifshitz-vdW model for 2D material stacks (supervised)
Outcomes: *Nat. Commun.* 2025, 16, 7726
Current position: CSL Switzerland

2017 - 2018 — Navanshu Ahuja (ETH Zürich, MSc Student)
Fabrication and analysis of orientation-induced F_{16}CuPc-graphene nanowire formation (supervised)
Outcomes: *Small* 2018, 14, 1870247
Current position: KPMG Switzerland

2016 — Raja Selvakumar (ETH Zürich, Visiting BSc Student from MIT)
Optimization of graphene-semiconductor interface fabrication (supervised)
Outcomes: *Small* 2018, 14, 1870247
Current position: PhD Student, GaTech, USA

Academic Service

Graduate Thesis Examining Committee

2025 - now — Graduate thesis examiners: 2

2025 - now — Graduate thesis committee chair: 3

University of Alberta Engineering AI Task Force (AITF)

2025 - 2026 — Committee member. Contributing to the strategic development of the faculty's undergraduate curriculum transition toward AI/ML.

Journal Reviewer

2022 - now — Journal of Open Source Software (JOSS), Scientific Reports, The European Physical Journal E, New Journal of Chemistry, RSC Advances, RSC Digital Discovery, APL Machine Learning, Nanomaterials (MDPI), Polymers (MDPI), Crystals (MDPI)

Teaching Experience

University of Alberta

2026 - **Graduate course**

MAT E 664 *Kinetics of Materials*

- Fundamental principles governing the rate and mechanisms of material processes
- Transport phenomena at material interfaces
- Time-dependent material change and evolution

2026 - **Undergraduate course**

CH E 318 *Mass Transfer*

- Fundamentals about mass transfer in chemical engineering
- Mass transfer coefficients
- Mass transfer equipment design

ETH Zürich

2016 - 2020 **Graduate course**

529-0610-01L *Interface Engineering of Materials* (TA)

- Interfacial phenomena of materials
- Electromagnetism origin of interfacial phenomena
- Numerical modelling of material interfaces

Academic Awards

2021 Chinese Government Award for Outstanding Self-Financed Students Abroad

2021 SNSF Early Postdoc.Mobility Fellowship

2019 SCNAT Chemistry Travel Award, Swiss Chemical Society

2014 Teijin Academic Scholarship (first-class academic scholarship)

2012 Outstanding Graduate Student of Tsinghua University

2012 Tsinghua School Scholarship for elite students

2011 First-class National Scholarship

2010 Third-class Academic Scholarship

2009 Dingye Mailin Academic Scholarship

Publications

[†]: Co-first author; [*]: Corresponding author

Journal Articles

1. Scalable Nanopatterning of OLEDs Beyond the Diffraction Limit
   Marcato, T.; Oh, J.; Lin, Z.-H.; **Tian, T.**; Gogoi, A.; Shivarudraiah, S. B.; Kumar, S.; Rajan, A. G.; Zeng, S.; Shih, C.-J.
   Nat. Photon. **2025**, *10*, accepted
2. Strong repulsive Lifshitz-van der Waals forces on suspended graphene
   Vagli, G.[†]; **Tian, T.**[†]; Naef, F.; Jinno, H.; Celebi, K.; Santos, E. J. G.; Shih, C.-J.
   Nat. Commun. **2025**, *16*, 7726 link
3. SPARC-X-API: Versatile Python Interface for Real-space Density Functional Theory Calculations
   Tian, T.[*]; Timmerman, L. R.; Kumar, S.; Comer, B.; Medford, A. J.; Suryanarayana, P.
   J. Open Source Softw. **2025**, *10*, 7747 link
4. Direct nanopatterning of complex 3D surfaces and self-aligned superlattices via molecular-beam holographic lithography
   Zeng, S.[†]; **Tian, T.**[†]; Oh, J.; Lin, Z.-H.; Shih, C.-J.
   Nat. Commun. **2025**, *16*, 3436 link
5. Lighting up aggregate emission of perylene diimide by leveraging polymerization-mediated through-space charge transfer and π-π stacking
   Ye, S.; Füglistaller, D.; **Tian, T.**; Manian, A.; Kumar, S.; Nardo, C.; Christofferson, A. J.; Russo, S. P.; Shih, C.-J.; Leroux, J.-C.; Bao, Y.
   Sci. China Chem. **2024**, *67*, 4218–4233 link
6. Adjusting Interface Dynamics: A New Insight into the Role of Electrolyte Additive in Facilitating Highly Reversible (002)-Textured Zinc Anode at High Current and Areal Densities
   Huang, H.; Xu, J.; Huang, Y.; He, Z.; Feng, H.; Hu, C.; Chen, Z.; Yang, Z.; **Tian, T.**[*]; Zhang, W.
   Adv. Energy Mater. **2024**, *14*, 2401643 link
7. Beyond independent error assumptions in large GNN atomistic models
   Ock, J.; **Tian, T.**; Kitchin, J.; Ulissi, Z.
   J. Chem. Phys. **2023**, *158*, 214702 link
8. Towards High-Performance Zinc Anode for Zinc Ion Hybrid Capacitor: Concurrently Tailoring Hydrodynamic Stability, Zinc Deposition and Solvation Structure via Electrolyte Additive
   Huang, H.; Yun, J.; Feng, H.; **Tian, T.**[*]; Xu, J.; Li, D.; Xia, X.; Yang, Z.; Zhang, W.
   Energy Storage Materials **2023**, *55*, 857–866 link
9. Machine learning-assisted exploration of a versatile polymer platform with charge transfer-dependent full-color emission
   Ye, S.; Meftahi, N.; Lyskov, I.; **Tian, T.**; Whitfield, R.; Kumar, S.; Christofferson, A. J.; Winkler, D. A.; Shih, C.-J.; Russo, S.; Leroux, J.-C.; Bao, Y.
   Chem **2023**, *9*, 924–947 link
10. FINETUNA: Fine-tuning Accelerated Molecular Simulations
    Musielewicz, J.; Wang, X.; **Tian, T.**; Ulissi, Z.
    Mach. Learn.: Sci. Technol. **2022**, *3*, 03LT01 link
11. Beyond conventional sodium-ion storage mechanisms: a combinational intercalation/conversion reaction mechanism in Ni-ion modified hydrated vanadate for high-rate sodium-ion storage
    Huang, H.; Wei, L.; **Tian, T.**[*]; Cao, T.; Cheng, F.; Chen, Z.; Yang, Z.; Ge, B.; Tian, M.; Zhang, W.; Niederberger, M.
    Energy Storage Mater. **2022**, *47*, 579–590 link
12. Continuous color tuning of single-fluorophore emission via polymerization-mediated through-space charge transfer
    Ye, S.; **Tian, T.**; Christofferson, A. J.; Erikson, S.; Jagielski, J.; Luo, Z.; Kumar, S.; Shih, C.-J.; Leroux, J.-C.; Bao, Y.
    Sci. Adv. **2021**, *7*, eabd1794 link
13. Electronic Polarizability as the Fundamental Variable in the Dielectric Properties of Two-Dimensional Materials
    Tian, T.; Scullion, D.; Hughes, D.; Li, L. H.; Shih, C.-J.; Coleman, J.; Chhowalla, M.; Santos, E. J. G.
    Nano Lett. **2020**, *20*, 841–851 link
14. Multifunctional Integrated Compartment Systems for Incompatible Cascade Reactions Based on Onion-like Photonic Spheres
    Zhou, K.; **Tian, T.**; Wang, C.; Zhao, H.; Gao, N.; Yin, H.; Wang, P.; Ravoo, B. J.; Li, G.
    J. Am. Chem. Soc. **2020**, *142*, 20605–20615 link
15. Amyloid fibril-templated high-performance conductive aerogels with sensing properties

Han, Y.; Cao, Y.; Bolisetty, S.; **Tian, T.**; Handschin, S.; Lu, C.; Mezzenga, R.
Small **2020**, *16*, 2004932 link

16. Multifunctional Nanoporous Polymer Membranes from Supramo-lecular Assembly of Block Copolymer with Polymerizable Arginine Derivative
Liang, Y.; Zhang, W.; **Tian, T.**; Ouyang, W.; Wang, P.; Wang, S.; Ju, Y.; Li, G.
Macromolecules **2020**, *53*, 1842–1851

17. Length- and Thickness-Dependent Optical Response of Liquid-Exfoliated Transition Metal Dichalcogenides
Synnatschke, K.; Cieslik, P. A.; Harvey, A.; Castellanos-Gomez, A.; **Tian, T.**; Shih, C.-J.; Chernikov, A.; Santos, E. J. G.; Coleman, J. N.; Backes, C.
Chem. Mater. **2019**, *31*, 10049–10062 link

18. Macroscopic Salt Rejection through Electrostatically Gated Nanoporous Graphene
Wyss, R. M.[†]; **Tian, T.**[†]; Yazda, K.; Park, H. G.; Shih, C.-J.
Nano Lett. **2019**, *19*, 6400–6409 link

19. Layered metal vanadates with different interlayer cations for high-rate Na-ion storage
Huang, H.; **Tian, T.**; Pan, L.; Chen, X.; Tervoort, E.; Shih, C.-J.; Niederberger, M.
J. Mater. Chem. A **2019**, *7*, 16109–16116 link

20. An Elastic Interfacial Transistor Enabled by Superhydrophobicity
Tian, T.; Sharma, C. S.; Ahuja, N.; Varga, M.; Selvakumar, R.; Lee, Y.-T.; Chiu, Y.-C.; Shih, C.-J.
Small **2018**, *14*, 1804006 link

21. Interfacial Field-Effect Transistors: An Elastic Interfacial Transistor Enabled by Superhydrophobicity (Small 51/2018, Cover Art)
Tian, T.; Sharma, C. S.; Ahuja, N.; Varga, M.; Selvakumar, R.; Lee, Y.-T.; Chiu, Y.-C.; Shih, C.-J.
Small **2018**, *14*, 1870247 link

22. Mixing Entropy-Induced Layering Polydispersity Enabling Efficient and Stable Perovskite Nanocrystal Light-Emitting Diodes
Kumar, S.; Jagielski, J.; **Tian, T.**; Kallikounis, N.; Lee, W.-C.; Shih, C.-J.
ACS Energy Lett. **2018**, *4*, 118–125 link

23. Monolayer Graphene Coupled to a Flexible Plasmonic Nanograting for Ultrasensitive Strain Monitoring
Tiefenauer, R. F.; Dalgaty, T.; Keplinger, T.; **Tian, T.**; Shih, C.-J.; Vörös, J.; Aramesh, M.
Small **2018**, *14*, 1801187 link

24. Spectroscopic Size and Thickness Metrics for Liquid-Exfoliated h-BN
Griffin, A.; Harvey, A.; Cunningham, B.; Scullion, D.; **Tian, T.**; Shih, C.-J.; Gruening, M.; Donegan, J. F.; Santos, E. J. G.; Backes, C.; Coleman, J. N.
Chem. Mater. **2018**, *30*, 1998–2005 link

25. Asymmetric electric field screening in van der Waals heterostructures
Li, L. H.; **Tian, T.**; Cai, Q.; Shih, C.-J.; Santos, E. J. G.
Nat. Commun. **2018**, *9*, 1271 link

26. Aggregation-induced emission in lamellar solids of colloidal perovskite quantum wells
Jagielski, J.; Kumar, S.; Wang, M.; Scullion, D.; Lawrence, R.; Li, Y.-T.; Yakunin, S.; **Tian, T.**; Kovalenko, M. V.; Chiu, Y.-C.; Lin, S.; Shih, C.-J.
Sci. Adv. **2017**, *3*, eaaq0208 link

27. Doping-Driven Wettability of Two-Dimensional Materials: A Multiscale Theory
Tian, T.; Lin, S.; Li, S.; Zhao, L.; Santos, E. J. G.; Shih, C.-J.
Langmuir **2017**, *33*, 12827–12837 link

28. Molecular Epitaxy on Two-Dimensional Materials: The Interplay between Interactions
Tian, T.; Shih, C.-J.
Ind. Eng. Chem. Res. **2017**, *56*, 10552–10581 link

29. Efficient Construction of Well-Defined Multicompartment Porous Systems in a Modular and Chemically Orthogonal Fashion
Gao, N.; **Tian, T.**; Cui, J.; Zhang, W.; Yin, X.; Wang, S.; Ji, J.; Li, G.
Angew. Chem. Int. Ed. **2017**, *129*, 3938–3943 link

30. Ultrapure Green Light-Emitting Diodes Using Two-Dimensional Formamidinium Perovskites: Achieving Recommendation 2020 Color Coordinates
Kumar, S.; Jagielski, J.; Kallikounis, N.; Kim, Y.-H.; Wolf, C.; Jenny, F.; **Tian, T.**; Hofer, C. J.; Chiu, Y.-C.; Stark, W. J.; Lee, T.-W.; Shih, C.-J.
Nano Lett. **2017**, *17*, 5277–5284 link

31. Wood Composites with Wettability Patterns Prepared by Controlled and Selective Chemical Modification of a Three-Dimensional Wood Scaffold
Wang, Y.; **Tian, T.**; Cabane, E.
ACS Sustainable Chem. Eng. **2017**, *5*, 11686–11694 link

32. Multiscale Analysis for Field-Effect Penetration through Two-Dimensional Materials
Tian, T.; Rice, P.; Santos, E. J. G.; Shih, C.-J.
Nano Lett. **2016**, *16*, 5044–5052 link

33. Chemically Patterned Inverse Opal Created by a Selective Photolysis Modification Process
Tian, T.; Gao, N.; Gu, C.; Li, J.; Wang, H.; Lan, Y.; Yin, X.; Li, G.
ACS Appl. Mater. Interfaces **2015**, *7*, 19516–19525 link

34. Helically structured metal–organic frameworks fabricated by using supramolecular assemblies as templates
Wang, H.; Zhu, W.; Li, J.; **Tian, T.**; Lan, Y.; Gao, N.; Wang, C.; Zhang, M.; Faul, C. F. J.; Li, G.
Chem. Sci. **2015**, *6*, 1910–1916 link

35. Metal-Organic Polyhedra Cages Immobilized on a Plasmonic Substrate for Sensitive Detection of Trace Explosives
Wang, C.; Shang, J.; Lan, Y.; **Tian, T.**; Wang, H.; Chen, X.; Gu, J.-Y.; Liu, J. Z.; Wan, L.-J.; Zhu, W.; Li, G.
Adv. Funct. Mater. **2015**, *25*, 6009–6017 link

36. AIE-induced fluorescent vesicles containing amphiphilic binding pockets and the FRET triggered by host–guest chemistry
Zhang, M.; Yin, X.; **Tian, T.**; Liang, Y.; Li, W.; Lan, Y.; Li, J.; Zhou, M.; Ju, Y.; Li, G.
Chem. Commun. **2015**, *51*, 10210–10213 link

37. Highly Sensitive Assay for Acetylcholinesterase Activity and Inhibition Based on a Specifically Reactive Photonic Nanostructure
Tian, T.; Li, X.; Cui, J.; Li, J.; Lan, Y.; Wang, C.; Zhang, M.; Wang, H.; Li, G.
ACS Appl. Mater. Interfaces **2014**, *6*, 15456–15465 link

38. Facile Fabrication of Reactive Plasmonic Substrates for Fluorescence Enhancement via Mussel-Inspired Chemistry
Wang, C.; Zhu, W.; Lan, Y.; Zhang, M.; **Tian, T.**; Wang, H.; Li, G.
J. Phys. Chem. C **2014**, *118*, 10754–10763 link

39. Self-assembled main-chain poly(bile acid) membranes that wrinkle
Li, W.; **Tian, T.**; Lan, Y.; Zhu, W.; Li, J.; Zhang, M.; Ju, Y.; Li, G.
Polym. Chem. **2014**, *5*, 743–751 link

40. Label-free detection and discrimination of poly-brominated diphenylethers using molecularly imprinted photonic cross-reactive sensor arrays
Xu, D.; Zhu, W.; Wang, C.; **Tian, T.**; Li, J.; Lan, Y.; Zhang, G.; Zhang, D.; Li, G.
Chem. Commun. **2014**, *50*, 14133–14136 link

41. Molecularly Imprinted Photonic Polymers as Sensing Elements for the Creation of Cross-Reactive Sensor Arrays
Xu, D.; Zhu, W.; Wang, C.; **Tian, T.**; Cui, J.; Li, J.; Wang, H.; Li, G.
Chem. Eur. J. **2014**, *20*, 16620–16625 link

42. Surface molecularly imprinted electrospun affinity membranes with multimodal pore structures for efficient separation of proteins
Zhu, T.; Xu, D.; Wu, Y.; Li, J.; Zhou, M.; **Tian, T.**; Jiang, Y.; Li, F.; Li, G.
J. Mater. Chem. B **2013**, *1*, 6449 link

43. Maleimide-containing polymer inverse opals: a new kind of reactive photonic structure with significant extendibility
Yang, H.; Li, X.; Lan, Y.; **Tian, T.**; Cui, J.; Zhu, T.; Shen, D.; Li, G.
J. Mater. Chem. C **2013**, *1*, 6120 link

44. Metal-free click approach for facile production of main chain poly(bile acid)s
Li, W.[†]; **Tian, T.**[†]; Zhu, W.; Cui, J.; Ju, Y.; Li, G.
Polym. Chem. **2013**, *4*, 3057 link

45. Reactive Photonic Film for Label-Free and Selective Sensing of Cyanide
Li, X.; Peng, L.; Cui, J.; Li, W.; Lin, C.; Xu, D.; **Tian, T.**; Zhang, G.; Zhang, D.; Li, G.
Small **2012**, *8*, 612–618 link

Conference Presentations

1. Machine Learning Models for Corrosion Mechanism Exploration (invited talk)
Tian, T.
AI in Corrosion & Integrity: AMPP Edmonton Chapter Technical Talk **2025**

2. Engineering 3D Nanopatterning via Molecular Beam Holographic Lithography
Tian, T.
35th Canadian Materials Science Conference (CMSC) **2024**

3. Transfer Learning of Graph Neural Networks As a General Approach to Accelerate Computational Catalysis Modeling
Tian, T.; Musielewicz, J.; Ock, J.; Ulissi, Z.
AIChE Annual Conference 2022 **2022**

4. Solid-state Lifshitz-van der Waals repulsion mediated by two-dimensional materials: Theories and observations
Tian, T.; Naef, F.; Vagli, G.; Celebi, K.; Li, Y.-T.; Chang, S.-W.; Krumeich, F.; Santos, E. J. G.; Chiu, Y.-C.; Shih, C.-J.
ACS Spring Meeting 2021 **2021** link

5. Unified understanding of the dielectric nature of 2D materials via electronic polarizability
Tian, T.; Scullion, D.; Santos, E.; Shih, C.-J.
Abstracts of Papers of the American Chemical Society **2019** link

6. Two-dimensional materials as high-pass filter of van der Waals interactions
Tian, T.; Naef, F.; Santos, E.; Shih, C.-J.
Abstracts of Papers of the American Chemical Society **2019** link

7. Multiscale analysis of the doping-driven wettability of two-dimensional materials
Tian, T.; Lin, S.; Li, S.; Zhao, L.; Santos, E.; Shih, C.-J.
Abstracts of Papers of the American Chemical Society **2019** link

8. Elastic interfacial transistor enabled by superhydrophobic self-assembled nanowires on graphene
Tian, T.; Chander, S.; Ahuja, N.; Varga, M.; Selvakumar, R.; Lee, Y.-T.; Chiu, Y.-C.; Shih, C.-J.
Abstracts of Papers of the American Chemical Society **2019** link

9. Macroscopic salt rejection through electrostatically gated nanoporous graphene
Tian, T.; Wyss, R.; Yazda, K.; Park, H. G.; Shih, C.-J.
Abstracts of Papers of the American Chemical Society **2019** link

10. Field effect transparency of 2D materials: A multiscale analysis
Tian, T.; Rice, P.; Santos, E.; Shih, C.-J.
Abstracts of Papers of the American Chemical Society **2018** link

11. Towards the understanding and engineering of the asymmetric electric field screening in van der Waals heterostructures
Li, L. H.; **Tian, T.**; Cai, Q.; Shih, C.-J.; Santos, E.
Abstracts of Papers of the American Chemical Society **2018** link

12. Modeling Gate-Tunable Ionic Transport Using Atomically Thin Patterned Graphene Membrane
Shih, C.-J.; **Tian, T.**; Wyss, R.; Yazda, K.; Park, H. G.
COMSOL Conference Collection **2018** link

13. Multiscale Approaches for Modeling the Penetration of Field Effect in Two-Dimensional-Materials-Based Quantum Capacitors
Tian, T.; Shih, C.-J.
2016 AIChE Annual Meeting Proceedings **2016** link

14. Maleimide-containing Responsive Photonic Crystal and Its Applications
Tian, T.; Gao, N.; Li, G.
5th International TRR61 Symposium, 2014, Suzhou, China

Open Source Contributions

2023 - now — SPARC | `SPARC-X/SPARC` (Github ☆ 70+)
Real-space *ab initio* quantum chemistry calculation package

2023 - now — SPARC-X-API | `SPARC-X/SPARC-X-API` (Github ☆ 10+)
Python API and driver for the SPARC QM code [paper link]

2021 - now — VaspInteractive | `ulissigroup/vasp-interactive` (Github ☆ 60+)
A stream-based calculator interface for VASP in high-throughput *ab initio* computations

2021 - now	FINETUNA	`ulissigroup/finetuna` (Github ☆ 50+) Fine-tuning accelerated molecular simulations powered by graph neural network. [paper link]
2021 - now	Beautiful Atoms	`beautiful-atoms/beautiful-atoms` (Github ☆ 100+) A python package for editing and rendering atomistic structures, powered by Blender.
2020	Simple Goniometer Interface (SGI)	`alchem0x2A/SGI` Open source user interface for contact angle goniometers, powered by Qt.
2019 - now	renishawWiRE	`alchem0x2A/py-wdf-reader` (Github ☆ 40+) Python parser for Renishaw Instrument's raman spectroscopy files
2018	Droplet-Pressure	`alchem0x2A/droplet_pressure` Numerical simulation for droplet shape and pressure evolution [paper link]