

Anna T. Bui

✉ btb32@cam.ac.uk annatbui.github.io

Education

- 2022 – **PhD in Theoretical Chemistry**, University of Cambridge, UK (expected Jun. 2026)
Working title: Statistical mechanics of solvation and transport in aqueous and ionic fluids
Advisor: Dr Stephen Cox
- 2018 – 2022 **BA (Hons) & MSci in Natural Sciences**, University of Cambridge, UK
1st Class, Rank 3/80
Thesis: Classical quantum friction at water–carbon interfaces
Advisors: Dr Stephen Cox and Prof Angelos Michaelides FRS

Other professional experience

- 2024 – **Visiting Graduate Researcher**, Department of Chemistry, Durham University, UK
- 2021 **Summer Undergraduate Researcher**, Yusuf Hamied Department of Chemistry, University of Cambridge, UK
Advisors: Prof Alex Thom and Prof Alex Forse
- 2019 **Summer Undergraduate Researcher**, Department of Materials Science, University of Cambridge, UK
Advisors: Dr Fabien Massabuau and Prof Rachel Oliver FREng

Awards, prizes and funding

Research

- 2022 – **Ernest Oppenheimer Graduate Scholarship**, School of the Physical Sciences, University of Cambridge
- 2022 – **Peterhouse Graduate Scholarship**, Peterhouse College, University of Cambridge
- 2025 **DCOMP Travel Award**, Division of Computational Physics, American Physical Society
- 2024 **RSC Poster Prize**, Faraday Community Poster Symposium, Royal Society of Chemistry
- 2024 **Best Talk Prize**, Showcase Day, Lennard–Jones Centre
- 2022 **IOP Poster Prize**, Advanced School in Liquids and Complex Fluids, Institute of Physics
- 2019 **Mason Fund**, Undergraduate Summer Research, Armourers and Brasiers

Academic

- 2019 – 2022 **Churchill College Scholarships**, Churchill College, University of Cambridge
- 2022 **Norrish Prize for Distinction in Physical Chemistry**, University of Cambridge
- 2021 **Katritzky Prize for Chemistry**, University of Cambridge
- 2019 **BP Prize for Chemistry**, University of Cambridge

Presentations

Upcoming

- 28. Dec. 2025 – Bristol Theoretical Physics Seminar, Bristol, UK (**Invited**)
- 27. Oct. 2025 – Stanford Theoretical Chemistry Seminar, hosted by Tom Markland, virtual (**Invited**)
- 26. Oct. 2025 – Chemistry Showcase Departmental Postgraduate Seminar, Cambridge, UK

Oral presentations

- 25. Sep. 2025 – Lennard-Jones Centre–CECAM: From electrons to atoms to molecules and materials, Cambridge, UK
"Learning classical density functionals for fluids" (**Invited**)
- 24. Aug. 2025 – The Chemistry and Physics of Liquids GRS, Holderness, NH, US:
"Liquid state theory in the 21st century: Electrolytes, electromechanics and dielectrocapillarity" (**Invited**)
- 23. Jul. 2025 – Oxford Soft Matter Seminar (hosted by Susan Perkin), Oxford, UK
"Liquid state theory in the 21st century: Electrolytes, electromechanics and dielectrocapillarity" (**Invited**)
- 22. Apr. 2025 – n-Aqua ERC synergy meeting (virtual):
"Momentum tunneling between nanoscale liquid flows" (**Invited**)
- 21. Apr. 2025 – 6th Multiscale Conference in biomolecular and condensed matter simulation, Manchester, UK:
"Learning classical density functionals for ionic and polar fluids"
- 20. Mar. 2025 – American Chemical Society Spring Meeting, San Diego, CA, US:
"Accurate descriptions of liquid–solid interfaces" (**Invited**)
- 19. Mar. 2025 – American Physical Society March Meeting, Anaheim, CA, US:
"Learning classical density functionals for ionic and polar fluids"
- 18. Jan. 2025 – Stanford University (hosted by Grant Rotskoff), CA, US:
"Faithful coarse-graining for solvation" (**Invited**)
- 17. Jan. 2025 – Pitzer Center for Theoretical Chemistry, UC Berkeley (hosted by David Limmer), CA, US:
"Faithful coarse-graining for solvation" (**Invited**)
- 16. Oct. 2024 – Lennard Jones Centre Showcase Day, Cambridge, UK:
"Learning classical density functionals for ionic fluids" (**Best Talk Prize**)
- 15. Nov. 2023 – Durham Centre for Soft Matter, Durham, UK:
"Solvation Across Length Scales: A Classical Density Functional Theory" (**Invited**)
- 14. Nov. 2023 – Departmental Theoretical Chemistry Seminar, Cambridge, UK:
"Solvation Across Length Scales: A Classical Density Functional Theory" (**Invited**)
- 13. Sep. 2023 – Faraday Discussions: Water at Interfaces, London, UK:
"Classical quantum friction at water–carbon interfaces" (**Selected Poster Presentation**)
- 12. Jul. 2023 – Nanofluidics in Physics and Biology, CECAM, Lyon, France:
"Classical quantum friction at water–carbon interfaces"
- 11. Jul. 2023 – n-Aqua ERC synergy project kick-off meeting (hosted by Mischa Bonn), Venice, Italy:
"Classical quantum friction and flow tunneling" (**Invited**)
- 10. Jun. 2023 – Young Researchers' School in Theory and Simulation in Electrochemical Conversion Processes, Paris, France:

"Classical quantum friction at water-carbon interfaces"

9. Apr. 2023 – Edwards Centre Celebration of Colloidal Sciences, Cambridge, UK:

"Hydrodynamics at the nanoscale: classical quantum friction and flow tunnelling" (**Invited**)

8. 2022–2024: Regular speaker at the [Chemistry Statistical Mechanics Meeting](#), Cambridge, UK

Poster presentations

7. Aug. 2025 – The Chemistry and Physics of Liquids GRC, Holderness, NH, US

"cDFT meets ML: A new era for liquid state theory"

6. Jan. 2025 – Berkeley Statistical Mechanics Meeting, Berkeley, CA, US:

"Learning classical density functionals for ionic fluids"

5. Dec. 2024 – Faraday Community Physical Chemistry Poster Symposium, London, UK:

"Liquid flows at the nanoscale" (**Best Poster Prize**)

4. Sep. 2024 – 12th Liquid Matter Conference, Mainz, Germany:

"A classical density functional theory for solvation across length scales"

3. Sep. 2024 – 8th Edwards Symposium: Statistical Physics of Soft and Multicomponent Systems, Cambridge, UK:

"A classical density functional theory for solvation across length scales"

2. Feb. 2023 – CECAM Mixed-Gen: Simulation and modelling of electrochemical interfaces and capacitors (virtual):

"Classical quantum friction at water-carbon interfaces"

1. Dec. 2022 – Advanced School in Liquids and Complex Fluids, Sheffield, UK:

"Classical quantum friction at water-carbon interfaces" (**Best Poster Prize**)

Teaching and Service

Research Supervision

2024 – 2025 Katie Zhou, Durham University, master's project & summer project

2024 Rebecca Driver, University of Cambridge, summer project

Undergraduate Teaching

2022 – 2024 Supervisor for third-year Theoretical Chemistry course, University of Cambridge

2022 – 2024 Demonstrator for second- and third-year Theoretical Chemistry practicals

Community building

2023 – Coordinator for the Lennard-Jones Centre Gender Equality Network
Organised Mentoring Scheme and Networking Events for women and non-binary researchers in molecular and materials modelling

Peer-reviewing

- Reviewed for *Journal of Chemical Physics*, *ACS Nano*, *Journal of Fluid Mechanics*, *Physical Review Letters*

Publications

* indicates publications with lead or co-lead authorship. Full list at: [Google Scholar](#)

Under review

- *12. **A. T. Bui** and S. J. Cox, [Dielectrocapillarity for exquisite control of fluids](#), *arXiv:2503.09855* (2025), in revision at *Nature Communications*
ATB developed the approach, wrote the algorithms, analysed results and wrote the paper

Peer-reviewed

- *11. **A. T. Bui** and S. J. Cox, [A first-principles approach to electromechanics in liquids](#), *Journal of Physics: Condensed Matter*, 37, 285101 (2025)
ATB developed the theory and wrote the paper
- *10. **A. T. Bui** and S. J. Cox, [Learning classical density functionals for ionic fluids](#), *Physical Review Letters*, 134, 148001 (2025)
ATB developed the approach, wrote the algorithms, analysed results and wrote the paper
- *9. B. Coquiot[†], **A. T. Bui**[†], D. Toquer, A. Michaelides, N. Kavokine, S. J. Cox, and L. Bocquet, [Momentum tunneling between nanoscale liquid flows](#), *Nature Nanotechnology*, 20, 397–403 (2025)
ATB designed and performed the simulations, analysed results and wrote the paper ([†] indicates co-lead authors)
- *8. **A. T. Bui** and S. J. Cox, [Revisiting the Green-Kubo relation for friction in nanofluidics](#), *Journal of Chemical Physics*, 161, 201102 (2024)
ATB developed the theory, performed the simulations, analysed results and wrote the paper
- *7. **A. T. Bui** and S. J. Cox, [A classical density functional theory for solvation across length scales](#), *Journal of Chemical Physics*, 161, 104103 (2024)
ATB developed the theory, wrote the algorithms, analysed results and wrote the paper
- *6. **A. T. Bui**, F. L. Thiemann, A. Michaelides and S. J. Cox, [Classical Quantum Friction at Water–Carbon Interfaces](#), *Nano Letters*, 23, 2, 580–587 (2023)
ATB designed and performed the simulations, analysed results and wrote the paper
- *5. **A. T. Bui**, N. A. Hartley, A. J. W. Thom and A. C. Forse, [Trade-Off between Redox Potential and the Strength of Electrochemical CO₂ Capture in Quinones](#), *Journal of Physical Chemistry C*, 126, 33, 14163–14172 (2022)
ATB designed and performed computational calculations, analysed results and wrote the paper
4. M. N. T. Anh, D. T. D. Nguyen, Y. C. Ching, N. V. K. Thanh, N. T. P. Phong, D. H. Nguyen, **A. T. Bui** and M.-T. Nguyen-Le, [Unveiling the SERS activity of silver triangular nanoplates in the enhanced detection of 4-mercaptobenzoic acid](#), *Optik*, 248, 168155 (2022)
ATB analysed results and wrote the paper

Proceedings

3. X. R. Advincula, K. E. Blow, M. Bonn, **A. T. Bui**, Y. Cheng, S. J. Cox, F. Della Pia, U. Diebold, L. Fumagalli, G. Goel, J. A. Hayton, Y. Jiang, V. Kapil, N. Kavokine, K. Koga, D. Laage, M. Lahav, S. Miao, A. Michaelides, P. Montero de Higes, K. Morgenstern, T. Mukherjee, N. O'Neill, D. Pan, P. M. Piaggi, S. L. B. Rempe, M. Salvalaglio, C. G. Salzmann, T. Sayer, M. Shepelenko, G. C. Sosso, S. Wang, B. Webber, A. P. Willard and Y. Yao, [Dynamics and nano-rheology of interfacial water: general discussion](#), *Faraday Discussions*, 249, 243–266 (2024)
2. E. H. G. Backus, G. Ben Ari, S. Benaglia, M. Bonn, **A. T. Bui**, S. J. Cox, F. Della Pia, J. Fraxedas, G. Goel, Y. Jiang, D. Jin, K. Koga, D. Laage, S. Miao, A. Michaelides, K. Morgenstern, T. Mukherjee, Y. Nagata, H. Naito, O. Nir, M. Olvera de la Cruz, H. Orlikowska-Rzeznik, D. Pan, S. L. B. Rempe, C. G. Salzmann, A. Taira, A. Vilangottunjalil, S. Wang, A. P. Willard, Y. Yao and J. Yu, [Soft matter–water interface: general discussion](#),

Faraday Discussions, 249, 485-520 (2024)

1. X. R. Advincula, E. H. G. Backus, T. Bartels-Rausch, S. Benaglia, G. Ben Ari, K. E. Blow, M. Bonn, **A. T. Bui**, S. J. Cox, F. Della Pia, U. Diebold, A. R. Finney, G. Franceschi, L. Fumagalli, G. Goel, J. A. Hayton, C. Holdship, Y. Jiang, D. Jin, V. Kapil, N. Kavokine, K. Koga, D. Laage, M. Lahav, S. Miao, A. Michaelides, N. Mohandas, K. Morgenstern, T. Mukherjee, Y. Nagata, M. Olvera de la Cruz, D. Pan, P. M. Piaggi, S. L. B. Rempe, P. Ryan, C. G. Salzmänn, T. Sayer, R. J. Saykally, M. Shepelenko, G. C. Sosso, T. F. Whale, J. J. White, A. P. Willard and P. Zhang, [Ice interfaces: general discussion](#), *Faraday Discussions*, 249, 133-161 (2024)