# Anna T. Bui

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## Research interests

My research uses statistical mechanics and computer simulations to model fluids' behaviours that often span across different length scales, capturing both microscopic correlations and mesoscopic phenomena. In my PhD, I focus on

- Equilibrium response: solvation phenomena, electric double layer
- Non-equilibrium response: how fluids flow under the nanoscale

My research heavily draws on theoretical techniques in soft matter (classical density functional theory, continuum hydrodynamics) and developing and applying them to systems of revelance in chemical physics (water, ions).

## Education

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| Oct 2022 – | **PhD in Theoretical Chemistry**, University of Cambridge, UK<br>Working title: Multiscale modeling of fluids in and out of equilibrium<br>Supervisor: Dr Stephen Cox |
| Oct 2018 – June 2021 | **BA & MSci in Natural Sciences**, University of Cambridge, UK<br>1st Class, Rank 3/80<br>Final year project: Classical quantum friction at water–carbon interfaces<br>Supervisors: Dr Stephen Cox and Prof Angelos Michaelides FRS |

## Other research experience

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| Sep 2024 – | **Visiting researcher**, Department of Chemistry, Durham University, UK<br>Supervisor: Dr Stephen Cox |
| June 2021 – Sep 2021 | **Summer intern**, Yusuf Hamied Department of Chemistry, University of Cambridge, UK<br>Supervisors: Dr Alex Thom and Prof Alex Forse |

## Awards, prizes, and funding

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| Oct 2022 – | **Ernest Oppenheimer Scholarship**, School of the Physical Sciences, University of Cambridge<br>Highly competitive studentship awarded (one or two each year) for research in Surface Chemistry and Physics, and Colloid Science [£124,000 / 3.5 years] |
| Oct 2022 – | **Peterhouse Graduate Studentship**, Peterhouse College, University of Cambridge<br>Competitive studentship awarded to scholars with highest academic calibre [£87,000 / 3 years] |
| Dec 2024 | **Poster prize**, Faraday Community Poster Symposium, Royal Society of Chemistry |
| Dec 2024 | **Best talk prize**, Showcase Day, Lennard–Jones Centre |
| Dec 2022 | **Poster prize**, Advanced School in Liquids and Complex Fluids, Institute of Physics |
| pre-2022 | **University of Cambridge**<br>Mason Fund, Armourers and Brasiers, funding for summer project [£4300]<br>Churchill College Scholarships [£480], Katritzky Prize for Chemistry [£400], Norrish Prize for Distinction in Physical Chemistry [£250], BP Prize for Chemistry [£200] |

## Publications

* indicate lead authorship

*6. **A. T. Bui**, and S. J. Cox, *arXiv:2410.02556, under review at PRL* (2024)
"Learning classical density functionals for ionic fluids"
*ATB developed the approach, wrote the algorithms, analysed results and wrote the paper*

*5. B. Coquinot*, **A. T. Bui***, A. Michaelides, N. Kavokine, S. J. Cox, and L. Bocquet, *Nature Nanotechnology* (2024)
"Momentum tunneling between nanoscale liquid flows"
*ATB designed and performed the simulations, analysed results and wrote the paper* (* indicates co-lead authors)

*4. **A. T. Bui**, and S. J. Cox, *Journal of Chemical Physics*, 161, 201102 (2024)
"Revisiting the Green-Kubo relation for friction"
*ATB developed the theory, performed the simulations, analysed results and wrote the paper*

*3. **A. T. Bui**, and S. J. Cox, *Journal of Chemical Physics*, 161, 104103 (2024)
"A classical density functional theory for solvation across length scales"
*ATB developed the theory, wrote the algorithms, analysed results and wrote the paper*

*2. **A. T. Bui**, F. L. Thiemann, A. Michaelides and S. J. Cox, *Nano Letters*, 23, 2, 580–587 (2023)
"Classical Quantum Friction at Water–Carbon Interfaces"
*ATB designed and performed the simulations, analysed results and wrote the paper*

*1. **A. T. Bui**, N. A. Hartley, A. J. W. Thom, and A. C. Forse, *Journal of Physical Chemistry C*, 126, 33, 14163–14172 (2022)
"Trade-Off between Redox Potential and the Strength of Electrochemical $CO_2$ Capture in Quinones"
*ATB designed and performed computational calculations, analysed results and wrote the paper*

## Presentations

**Oral presentations**

8. Oct 2024 – Lennard Jones Centre Showcase Day, Cambridge, UK:
*"Learning classical density functionals for ionic fluids"* (**Best Talk Prize**)
7. Nov 2023 – Durham Centre for Soft Matter, Durham, UK:
*"Solvation Across Length Scales: A Classical Density Functional Theory"*
6. Nov 2023 – Departmental Theoretical Chemistry Seminar, Cambridge, UK:
*"Solvation Across Length Scales: A Classical Density Functional Theory"*
5. July 2023 – Nanofluidics in Physics and Biology, CECAM, Lyon, France:
*"Classical quantum friction at water–carbon interfaces"*
4. July 2023 – *n-Aqua ERC synergy project kick-off meeting*, Venice, Italy:
*"Classical quantum friction and flow tunneling"*
3. June 2023 – *Researchers' School in Theory and Simulation in Electrochemical Conversion Processes*, Paris, France:
*"Classical quantum friction at water–carbon interfaces"*
2. April 2023 – Edwards Centre Celebration of Colloidal Sciences, Cambridge, UK:
*"Hydrodynamics at the nanoscale: classical quantum friction and flow tunnelling"* (**Invited**)
1. Regular speaker at the *Statistical Mechanics Seminar*, Cambridge, UK

**Poster presentations**

6. Dec 2024 – Faraday Community Physical Chemistry Poster Symposium, London, UK:
*"Liquid flows at the nanoscale"* (**Best Poster Prize**)
5. Sep 2024 – 12th Liquid Matter Conference, Mainz, Germany:
*"A classical density functional theory for solvation across length scales"*
4. Sep 2024 – 8th Edwards Symposium: Statistical Physics of Soft and Multicomponent Systems, Cambridge, UK:
*"A classical density functional theory for solvation across length scales"*
3. Sep 2023 – Faraday Discussions: Water at Interfaces, London, UK:

*"Classical quantum friction at water–carbon interfaces"*

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 experience

2024 – **Supervisions of research projects**
Day-to-day supervisor for a 16-week undergraduate research project (Durham)
Day-to-day supervisor for an 8-week summer undergraduate research project (Cambridge)

2022 – 2024 **Undergraduate teaching**
Supervisor for third-year theoretical chemistry course (Cambridge)
Laboratory demonstrator for second and third year theoretical chemistry course (Cambridge)

## Administrative duties

2023 – **Lennard Jones Centre Gender Equality Network coordinator**
Organisor of mentoring scheme for female and non-binary researchers within the molecular and materials modelling field