

# Charles Harris

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## EDUCATION

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**University of Cambridge** Oct. 2021 – Present  
*PhD in Computer Science* Cambridge, UK

- **Research:** Focus on molecular design, diffusion models and structure-based drug design
- **Supervisors:** [Prof Sir Tom Blundell](#), [Prof Pietro Liò](#)

**Imperial College London** Oct. 2020 – Sept. 2021  
*MSc in Bioinformatics and Theoretical Systems Biology - **Distinction - 76.5%*** London, UK

- **Supervisors:** [Prof Michael Bronstein](#) (Oxford, Twitter), [Prof Bruno Correia](#) (EPFL), [Prof Michael Sternberg](#)

**Imperial College London** Oct. 2017 – Sept. 2020  
*BSc in Biochemistry - 2:1* London, UK

- **Core modules:** Structural Biology, Drug Design, Bioinformatics, Systems Biology

## EXPERIENCE

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**British Government, UK Sovereign AI Unit** Mar. 2025 - Present  
*Technical Lead* London, UK

- First and only technical expert in the new SovAI unit, responsible for ensuring the UK has a stake in the future of AI
- Focusing on delivering the AI for Science component of the [AI Action Plan](#) with Matt Clifford
- Originated and led the Units 8m anchor investment into OpenBind, a dataset initiative for AI-driven drug discovery
- Identified and led a 5m expansion of the Encode AI for Science Fellowship, doubling its size and reach
- Evaluated the first batch of compute allocation into major AI projects on the national GPU cluster (>2.5m H200 hours)

**IQ Captical** Jun. 2024 – Sep. 2024  
*Venture Fellow* London, UK

**BenevolentAI** Jul. 2022 – Sept. 2022  
*AI Scientist Intern* London, UK

- Performed research on new AI tools using GNNs and self-supervised learning for the Target Identification team.

## PUBLICATIONS

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**TABASCO: A Fast, Simplified Model for Molecular Generation with Improved Physical Quality.** C. Vonessen\*, **C. Harris\***, M. Cretu\*, P. Lio - *Under review at NeurIPS 2025.* [Link](#)

**Straight but not so fast: Challenges with Rectified Flows in Protein Design.** J. Chen, S. Mathis, **C. Harris**, K. Didi, P. Lio - *ICML 2025 GenBio Workshop.* [Link](#)

**Diffusion-Free Graph Generation with Next-Scale Prediction.** S. Belkadi, S. Hong, M Chen, M. Cretu,, **C. Harris**, P. Lio - *ICML 2025 GenBio Workshop.* [Link](#)

**Structure-based Generation of a Secondary Nucleation Inhibitor in  $\alpha$ -synuclein Aggregation using a Conditional Diffusion Model.** H. Zhang, R. I. Horne, Z. F. Brotzakis, **C. Harris**, P. Lio, M. Vendruscolo - *Under review at Science Advances.*

**SynFlowNet: Towards Molecule Design with Guaranteed Synthesis Pathways.** M. Cretu, **C. Harris**, I. Igashov, A. Schneuing, M. Segler, B. Correia, J. Roy, E. Bengio, P. Lio - *ICLR 2025 (Spotlight)*. [Link](#)

**Multi-State RNA Design with Geometric Multi-Graph Neural Networks.** C. Joshi, A. Jasamb, R. Vinas **C. Harris**, S. Mathis, P. Lio - *ICLR 2025 (Spotlight)*. [Link](#)

**Equivariant Diffusion Models for Structure-based Drug Design.** A. Schneuing\*, **C. Harris\***, Y. Du\*, A. R. Jamasb, I. Igashov, W. Du, T. L. Blundell, P. Lió, C. Gomes, M. Welling, M. Bronstein, B. Correia. - *Nature Computational Science 2024*. [Link](#)

**Machine Learning-aided Generative Molecular Design.** Y. Du\*, A. R. Jamasb\*, J. Guo\*, T. Fu<sup>+</sup>, **C. Harris<sup>+</sup>**, Y. Wang, C. Duan, P. Lio, P. Schwaller, T. Blundell. *Nature Machine Intelligence*. [Link](#)

**RNA-FRAMEFLOW for de novo 3D RNA Backbone Design** R. Anand, C. Joshi, A. Morehead, A. Jamasb, **C. Harris**, S. Mathis, K. Didi, B. Hooi, P. Lio. *TMLR 2025*. [Link](#)

**Evaluating Representation Learning on the Protein Structure Universe** A. Jamasb, A. Morehead, Z. Zhang, C. Joshi, K. Didi, S. Mathis, **C. Harris**, J. Tang, J. Cheng, P. Lio, T. Blundell - *ICLR 2024*.

**PoseCheck: Generative Models for 3D Structure-based Drug Design Produce Unrealistic Poses.** **C. Harris**, K. Didi, A. Jamasb, C. Joshi, S. Mathis, P. Lio, T. Blundell - *NeurIPS 2023 MLSB Workshop* - [Oral]. [Link](#)

**DiffHopp: A Graph Diffusion Model for Novel Drug Design via Scaffold Hopping.** J. Torge, **C. Harris**, S. Mathis, P. Lio - *ICML WCB 2023* - [Spotlight]. [Link](#)

**Flexible Small-Molecule Design and Optimization with Equivariant Diffusion Models.** **Charles Harris**, K. Didi, A. Schneuing, Y. Du, A. Jamasb, M. Bronstein, B. Correia, P. Lio, T. Blundell - *ICLR MLDD 2023*. [Link](#)

**Graphain - a Python Library for Geometric Deep Learning and Network Analysis on Protein Structures and Interaction Networks.** A. R. Jamasb, R. Viñas Torné, E. J. Ma, **C. Harris**, K. Huang, D. Hall, P. Lió, T. L. Blundell. - *NeurIPS 2022*. [Link](#)

## COMMUNICATION

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### Blogs: Charlie's Substack

Articles on AlphaFold3 and 100+ TechBio company database (200+ subscribers)

[Link](#)

Jul. 2022 - Present

### Guest Writer - Royal Society of Chemistry CICAG Newsletter

Published articles on AI in Drug Discovery and Diffusion Models (viewed over 5,000 times)

[Article](#)

Ongoing

### Chair and Founder - 1st Cambridge AI in Drug Discovery Conference

Sold over 3,000 tickets

[Event website](#)

Feb. 2022

### Guest - iGEM Synthetic Biology Podcast

Discussed AlphaFold2, my research and the impact of computation and AI on biology in general

[Link](#)

Aug. 2021

### Chair and Founder - 1st Imperial AI in Drug Discovery Conference

Sold over 1,400 tickets

[Handbook](#)

Feb. 2021

- Created and chaired Imperial's first **AI in Drug Discovery Conference** with top scientists, business leaders and entrepreneurs, over 1,400 tickets sold
- Moderated two panel discussions (first one with 4 CEOs/Founders of AI in Drug Discovery companies and second with Prof Sir Tom Blundell, Prof Michael Bronstein and Dr Andreas Bender)

## INVITED TALKS

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<b>Graph Neural Networks and Geometric Deep Learning Course</b> - <i>University of Cambridge</i>	Feb. 2025
<b>British Ambassadors Residence</b> - <i>Rome, Italy</i>	Nov. 2024
<b>Department of Computer Engineering, Sapienza University of Rome</b> - <i>Rome, Italy</i>	Feb. 2024
<b>VantAI "AI in Drug Discovery Seminar Series"</b> - <i>NYC, USA</i> - <u>Recording</u>	Nov. 2023
<b>AstraZeneca AI Journal Club</b> - <i>Cambridge, UK</i>	Aug. 2023
<b>Genesis Therapeutics</b> - <i>San Francisco, USA</i>	Aug. 2023
<b>Merck</b> - <i>San Francisco, USA</i>	Aug. 2023
<b>Cambridge Chemoinformatics Network meeting</b> - <i>University of Cambridge</i> - <u>Recording</u>	Jun. 2023
<b>Imperial College Computational Biology Conference</b> - <i>Imperial College London</i>	May 2023
<b>AstraZeneca</b> - <i>Cambridge, UK</i>	April 2023
<b>IBM Research</b> - <i>Zurich, Switzerland</i>	April 2023
<b>AI UK Conference (Demonstrator)</b> - <i>QEI Conference Centre, Westminster</i>	Mar. 2023
<b>Graph Neural Networks and Geometric Deep Learning Course</b> - <i>University of Cambridge</i>	Feb. 2023

## SUPERVISING

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<b>Jos Torge - Part III Computer Science Tripos Project</b> <i>Generative models for enzymatic functional motif design</i>	Jan. 2025 – Present
<b>Junhua Chen - MPhil Computer Science Project</b> <i>SE(3) ReFlow for efficient flow-matching models for protein design</i>	Jan. 2025 – Present
<b>Carlos Vonessen (ETH Zurich) - Visiting Masters Project</b> <i>Reaction-conditioned diffusion models for synthesisable SBDD</i>	Jan. 2025 – Present
<b>Krisztina Sinkovics - MPhil Machine Learning</b> <i>Theory of conditional flow-matching for small molecule design</i>	76% Jan. 2024 – Sep. 2024
<b>Jamie Weigold (now CEO of Empirical) - MPhil Computer Science Project</b> <i>Diffusion models for protein-protein docking</i>	87.5% - Top 3 project in cohort Oct. 2022 – Jul. 2023
<b>Keiran Didi - MPhil Computational Biology Project</b> <i>Diffusion models for the protein motif-scaffolding problem</i>	90% - Top project in cohort Oct. 2022 – Jul. 2023
<b>Jos Torge - Part II Computer Science Tripos Project</b> <i>DiffHopp: A Graph Diffusion Model for Novel Drug Design via Scaffold Hopping</i>	<u>Spotlight paper at WCB ICML 2024</u> Oct. 2022 – Jul. 2023
<b>Mihailo Milosevic - Part II Computer Science Tripos Project</b> <i>Self-supervised learning of ligand-binding</i>	Oct. 2022 – Jul. 2023
<b>Keval Shah - Part III Computer Science Tripos Project</b> <i>Self-supervised learning of ligand-binding</i>	81% Oct. 2021 – Jul. 2022
<b>Zhang Shu - MPhil Computational Biology Project</b> <i>Equivariant denoising diffusion models for protein ligand binding</i>	Jan. 2022 – Jul. 2022
<b>Olivier Dietrich - Visiting Masters Project</b> <i>AI for enzyme kinetics predictions using multi-modal representations</i>	Jan. 2022 – Jul. 2022

## ACADEMIC SERVICE

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### Organiser

*Machine Learning for Life and Material Sciences Workshop at ICML 2024* Feb. 2024 – July. 2024

### Reviewer

*Machine Learning for Structural Biology Workshop at NeurIPS 2023* Feb. 2024 – July. 2024

## Reviewer

*Computational Biology Workshop at ICML 2023*

Feb. 2024 – July. 2024

## Mentor/Organiser

*Catalyse Competition - [SynBioUK](#)*

Dec. 2020 – Present

## Advisor

*Imperial College International Directed Evolution Competition (iDEC) Team*

[Project Website](#)  
Jun. 2021 – Oct. 2021

- Advised the team on how to leverage different protein structure prediction tools for their project (including AlphaFold2)

## TEACHING

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**Geometric Deep Learning - Part III/MPhil CS, University of Cambridge**  
**Bioinformatics - Part II Computer Science Tripos, University of Cambridge**

Jan. 2022 - Present  
Nov. 2021 - Dec. 2021

## AWARDS - ACADEMIC

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**Venture Fellowship** - IQ Capital  
**Polaris Fellowship** - Entrepreneur First  
**UK-Italy Visiting Researcher Fellowship** - Alan Turing Institute  
**CCAIM PhD Studentship** - University of Cambridge  
**Associateship** - Royal College of Science  
**Gold** - UK Chemistry Olympiad  
**Prefect** - Leighton Park School  
**David Lean Scholar** - Leighton Park School

Jun. 2024  
Dec. 2023  
Oct. 2023  
Oct. 2021  
Jul. 2020  
Jun. 2017  
June. 2016  
Sep. 2015

## AWARDS - SPORTING

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**Cambridge Half Blue (Gliding)** - University of Cambridge  
**1st Place** - Oxford-Cambridge Gliding Varsity  
**1st Place, Best Technical Soaring Flight** - National Interuniversity Gliding Competition

July. 2023  
July. 2023  
July. 2023

## VOLUNTEERING

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### Ordinary Committee Member

*Cambridge University Gliding Club*

May. 2022 – Jan. 2024

### Events and Conference Officer

*Cambridge University Artificial Intelligence Society*

[Website](#)  
Oct. 2021 – Oct. 2022

### Chair and Founder

*Imperial College Computational Biology Society*

[Twitter](#) - [Instagram](#)  
Oct. 2019 – Aug. 2021

### Ambassador

*Helen Arkell Dyslexia Charity*

Oct. 2019 – Present

## OTHER SKILLS

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**Languages:** Mandarin (A at GCSE Level)

**Interests:** Qualified glider pilot (Full Silver Badge, 1st Place - Oxford-Cambridge Varsity 2023), Hockey, Running, Drone photography, Science communication