Charles Harris

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EDUCATION

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

- **Research**: Focus on molecular design, generative AI and discovering new biology with self-supervised learning
- **Supervisors**: Prof Sir Tom Blundell, Prof Pietro Liò
- **Funding**: Cambridge Centre for AI in Medicine (CCAIM) Studentship, sponsored by AstraZeneca and GSK

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

BenevolentAI July. 2022 – Sept. 2022
AI Scientist Intern London, UK

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

Cambridge Centre for AI in Medicine Oct. 2021 – Present
PhD Student Cambridge, UK

PUBLICATIONS

Benchmarking Generated Poses: How Rational is Structure-based Drug Design with Generative Models?. C. Harris, K. Didi, A. Jamasb, C. Joshi, S. Mathis, P. Lio, T. Blundell - *Under review*.

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

Multi-State RNA Design with Geometric Multi-Graph Neural Networks. C. Joshi, A. Jasamb, R. Vinas **C. Harris**, S. Mathis, P. Lio - *ICML WCB 2023*.

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 Workshop 2023*. Link

Equivariant Diffusion Models for Structure-based Drug Design. A. Schneuing, Y. Du, **C. Harris**, A. R. Jamasb, I. Igashov, W. Du, T. L. Blundell, P. Lió, C. Gomes, M. Welling, M. Bronstein, B. Corriea. - *NeurIPS MLSB Workshop 2022*. Link

Graphein - 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

TECHNICAL SKILLS

Deep Learning: PyTorch, PyTorch Geometric, PyTorch Lightning, Keras, some experience with JAX
Computing: Linux, AWS, Kubernetes, SQL, GPU machines, computing clusters
Cloud computing: Docker, AWS, Kubeflow, Kubernetes
Structural Biology: Deep understanding of protein structure. Highly proficient in PyMol and structure prediction
Chemoinformatics/drug design: RDKit, Conventional docking (AutoDock, SWISSDOCK)
Biochemistry and molecular biology: Strong background in and understanding of common lab data collect techniques

COMMUNICATION

Guest Writer - Royal Society of Chemistry CICAG Newsletter Article
Published article on AI in Drug Discovery and soon to have article on Diffusion Models Feb. 2022

Chair and Founder - 1st Cambridge AI in Drug Discovery Conference Event website
Sold over 3,000 tickets Feb. 2022

Guest - iGEM Synthetic Biology Podcast Link
Discussed AlphaFold2, my research and the impact of computation and AI on biology in general Aug. 2021

Chair and Founder - 1st Imperial AI in Drug Discovery Conference Handbook
Sold over 1,400 tickets Feb. 2021

- 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

Cambridge Chemoinformatics Network meeting - *University of Cambridge - Link* June. 2023
Imperial College Computational Biology Conference - *Imperial College London* May 2023
AstraZeneca - *Cambridge* April 2023
IBM Research - *Zurich* April 2023
AI UK Conference (Demonstrator) - *QEII Conference Centre, Westminster* Mar. 2023
Graph Neural Networks and Geometric Deep Learning Course - *University of Cambridge* Feb. 2023
Machine Learning for Structural Biology Workshop (Poster) - *NeurIPS 2022* Dec. 2022
Sidney Sussex College Graduate Research Conference - *University of Cambridge* May. 2022

ADVISORY POSITIONS

Advisor - *Cambridge University International Genetically Engineered Machine (iGEM) Team* Dec. 2021 - Mar. 2022
Advisor - *Imperial College International Directed Evolution Competition (iDEC) Team* Jun. 2021 - Oct. 2021
Mentor/Organiser - *Catalyse Competition - SynBioUK* Dec. 2020 - Oct. 2021

TEACHING

Representation Learning on Graphs/Networks - *Part III/MPhil CS, University of Cambridge* Jan. 2022 - Present
Bioinformatics - *Part II Computer Science Tripos, University of Cambridge* Nov. 2021 - Dec. 2021

AWARDS

CCAIM PhD Studentship - *University of Cambridge* Oct. 2021
Associateship - *Royal College of Science* Jul. 2020
Gold - *UK Chemistry Olympiad* Jun. 2017
Prefect - *Leighton Park School* June. 2016
David Lean Scholar - *Leighton Park School* Sep. 2015

VOLUNTEERING

Events and Conference Officer Website
Cambridge University Artificial Intelligence Society Oct. 2021 – Present

Chair and Founder Twitter - Instagram
Imperial College Computational Biology Society Oct. 2019 – Aug. 2021

Ambassador
Helen Arkell Dyslexia Charity Oct. 2019 – Present

OTHER SKILLS

Languages: Mandarin (A at GCSE Level)
Interests: Qualified glider pilot (Silver Badge), Hockey, Running, Drone photography, Science communication