

# Charles Harris

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## EDUCATION

### University of Cambridge

*PhD in Computer Science and Technology*

Oct. 2021 – Present

Cambridge, UK

- **Supervisors:** [Prof Pietro Liò](#), [Prof Sir Tom Blundell FRS](#),
- **Funding:** Cambridge Centre for AI in Medicine ([CCAIm](#)) Studentship, sponsored by [AstraZeneca](#) and [GSK](#)

### Imperial College London

*MSc in Bioinformatics and Theoretical Systems Biology - **Distinction***

Oct. 2020 – Sept. 2021

London, UK

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

### Imperial College London

*BSc in Biochemistry - 2:1*

Oct. 2017 – Sept. 2020

London, UK

## SELECTED PROJECTS

### MSc Project 3 - Distinction

Supervisors: Prof Michael Bronstein, Prof Bruno Correia

*Geometric Deep Learning for structure-based drug design*

Jun. 2021 – Sept. 2021

- Developed a molecular graph generation procedure which improves previous work by conditioning multiple stages of the generative procedure with an attention mechanism between the molecule and protein pocket (using [dMaSIF](#))

### MSc Project 2 - Distinction

Supervisors: Michael Bronstein, Bruno Correia

*Learning interpretable protein dynamics using Geometric Deep Learning*

Apr. 2021 – Jun. 2021

- Created a novel message-passing layer for protein graphs that learns interpretable protein dynamics

### MSc Project 1 - Distinction

Supervisor: Prof Michael Sternberg

*Prediction of the effect of missense variants involved in ligand binding via docking*

Jan. 2021 – April. 2021

### Graphene - Open Source Contributor - Preprint

*Graphene aims to democratise access to protein graph data for geometric deep learning models*

## PREPRINTS

**Graphene - 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., [preprint](#)

## TECHNICAL SKILLS

**Python:** PyTorch, PyTorch Geometric, Deep Graph Library/DGL-LifeSci, NetworkX, Tensorflow/Keras, some experience with Sonnet and JAX/Jraph

**Computing:** Linux, SQL, GPU machines, familiar with use of computing clusters

**Statistics:** Proficient in R, Probability, Likelihood statistics, Bayesian statistics, Linear regression, Classification

**Structural Biology:** Deep understanding of protein structure. Highly proficient in PyMol. Highly experienced in structure prediction (AlphaFold2, Phyre2) Experience with building atomic models in Coot and NMR analysis in CCPNmr

**Chemoinformatics/drug design:** RDKit, Conventional docking (AutoDock, SWISSDOCK)

**Biochemistry and molecular biology:** Strong background in and understanding of common lab data collect techniques

**Bioinformatics:** Genome assembly and annotation, RNA-seq data analysis, Sequence alignment, Protein function and structure prediction, NGS data analysis in R and Artemis

**Systems biology/MatLab:** ODEs, Master equations, Gillespie simulations, Dynamical systems (linear stability analysis, bistability, phase portraits), Quantitative cell imaging

## SCIENCE COMMUNICATION

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

*Chaired multiple talks and discussion panels from scientific and business leaders - see [handbook](#)*

Feb. 2021

### Guest - iGEM Synthetic Biology Podcast

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

[Link](#)

Aug. 2021

## VOLUNTEERING

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### Advisor

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

Jun. 2021 – Oct. 2021

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

### Chair and Founder

*Imperial College Computational Biology Society*

Oct. 2019 – Aug. 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 as part of conference (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)
- Organised regular webinar schedule with top companies and academics in computational biology (including BenevolentAI/Dr Nathan Brown, DeepMind (Dr Petar Velikovi) Nvidia, LabGenius, Imperial and UCL)
- Organised six workshops to teach biologist computational and coding skills
- Quickly grew the Society to over 340 members and developed a strong social media presence
- Showed strong leadership, organisational and team building skills by creating an effective team and culture from scratch. Managed 20 volunteers and numerous projects in the first term

### Ambassador

*Helen Arkell Dyslexia Charity*

Oct. 2019 – Present

### Secretary

*Imperial College Amnesty International Society*

Oct. 2019 – Aug. 2020

## REFERENCES - all are past and present supervisors

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### Prof Sir Tom Blundell FRS - University of Cambridge

[tom@cryst.bioc.cam.ac.uk](mailto:tom@cryst.bioc.cam.ac.uk)

*Professor Emeritus of Biochemistry, Former President - BBSRC, Biochemical Society*

### Prof Peitro Lio - University of Cambridge

[pl219@cam.ac.uk](mailto:pl219@cam.ac.uk)

*Professor of Computational Biology. Member - Artificial Intelligence Group and CCAIM*

### Prof Michael Bronstein - Imperial College London, Twitter

[m.bronstein@imperial.ac.uk](mailto:m.bronstein@imperial.ac.uk)

*Chair of Machine Learning at Imperial, Head of Graph Learning Research at Twitter*

### Prof Michael Sternberg FRSB - Imperial College London

[m.sternberg@imperial.ac.uk](mailto:m.sternberg@imperial.ac.uk)

*Director - Centre for Integrative Systems Biology and Bioinformatics*

### Prof Bruno Correia - EPFL

[bruno.correia@epfl.ch](mailto:bruno.correia@epfl.ch)

*Head - Laboratory of Protein Design and Immunoengineering*

## OTHER SKILLS

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**Awards:** Gold - International Chemistry Olympiad 2017 UK Round 1, David Lean Scholar and Prefect - Leighton Park

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

**Interests:** Glider pilot, Hockey, Running, Drone photography, Science communication