Chaitanya K. Joshi

Curriculum vitæ (6th February 2025)

Ph.D. Student
Department of Computer Science & Technology
Clare Hall College
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Chaitanya K. Joshi
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Education

01/2022–present **University of Cambridge, UK**, Ph.D. in Computer Science.
Qualcomm Innovation Fellow, A*STAR National Science Scholar.
Geometric Deep Learning for Biomolecule Design; supervisor: Prof. Pietro Liò.

07/2015–05/2019 **Nanyang Technological University, Singapore**, B.Eng. in Computer Science.
Valedictorian, Best Thesis Gold Medal, Best Internship Award, Dean's List ×2.
Graph Neural Networks for the Travelling Salesman Problem; supervisor: Prof. Xavier Bresson.

Work Experience

02/2025–05/2025 **Visiting Researcher, MRC Laboratory of Molecular Biology**, Cambridge, UK.
Phil Holliger's Lab, Protein and Nucleic Acid Chemistry division.

07/2024–09/2024 **Research Scientist Intern, Fundamental AI Research (FAIR), Meta**, San Francisco, California, USA.
FAIR Chemistry Team. Generative models for molecules and materials, with Dr. Zachary Ulissi.

07/2023–09/2023 **Research Scientist Intern, Genentech, Roche**, Basel, Switzerland.
Prescient Design Team. Geometric GNNs for protein molecular dynamics, with Dr. Andreas Loukas.

07/2020–12/2021 **Research Engineer, Institute for Infocomm Research, A*STAR**, Singapore.
Resource-efficient Graph Neural Networks, with Dr. Chuan Sheng Foo and Dr. Lin Jie.

07/2019–07/2020 **Research Assistant, Graph Deep Learning Lab, NTU**, Singapore.
Graph Neural Networks and applications to combinatorial optimisation, with Prof. Xavier Bresson.

Honours & awards

2024
- **Qualcomm Innovation Fellowship**, value: USD 40,000, top 5 PhD students across Europe.
- **Wiseman Prize, Department of Computer Science, University of Cambridge**. For commendable contributions to the department (supervision, teaching, organizing lab socials).
- **Cambridge HPC Pioneer Project grant**, awarded to pilot *Dawn*, UK's new AI supercomputer; value: 10,000 GPU hours.
- **Top Reviewer Awards** at ICML 2024, NeurIPS 2022, ICLR 2022, NeurIPS 2021.

2023
- **Accelerate Science & Cambridge Centre for Data-Driven Discovery grant**, to host the conference *Understanding Biology in the age of AI* held in Cambridge, UK in June 2023; value: 14,000 GBP.

2021
- **National Science Scholarship, A*STAR, Singapore**. Fully funded scholarship to pursue PhD studies at University of Cambridge, UK; value: USD 800,000, 5 years of research funding.

2019
- **Valedictorian, School of Computer Science & Engineering, NTU, Singapore**.
Awarded for excellent academic performance, leadership qualities and public-speaking skills among the graduating cohort. Valedictory speaker for Class of 2019.
- **Best Final Year Thesis Gold Medal**, NTU, Singapore, for B.Eng. thesis with Prof. Xavier Bresson.

2018
- **Best Professional Internship Award**, NTU, Singapore, for Research Internship at SAP.

Presentations & Invited talks

Most talks and slides are available via my YouTube channel (13K+ total views).

- **gRNAde: Geometric Deep Learning for 3D RNA Inverse Design**.
  - 01/2025 RNA Nanotechnology Gordon Research Seminar, USA.
  - 08/2024 Department of Biochemistry, Stanford University, USA, host: Prof. Rhiju Das.
  - 06/2024 Jeffrey Cheah Biomedical Centre, University of Cambridge, UK; host: Cambridge AI-Biomedicine Club.
  - 04/2024 Department of Computer Science, NUS, Singapore, host: Prof. Yang Zhang.
  - Genome Institute of Singapore, A*STAR, host: Dr. Yue Wan.
  - Institute of Molecular and Cell Biology, A*STAR, Singapore, host: Dr. Sherry Aw.
  - 03/2024 Roche, Advanced Analytics Network Conference, Basel, Switzerland, host: Dr. Igor Kulev.
  - 01/2024 CASP RNA Special Interest Group, host: Dr. Marcin Magnus (Harvard), Rachael Kretsch (Stanford).
  - 11/2023 NUS Yong Loo Lin School of Medicine, Singapore, host: Prof. Roger Foo.
  - 10/2023 MRC Laboratory of Molecular Biology, host: Dr. Phil Holliger.

- **On the Expressive Power of/A Hitchhiker's Guide to Geometric Graph Neural Networks**.
  - 01/2024 Department of Computer Science, IIT Delhi, India, host: Prof. Sayan Ranu.
  - 05/2023 Mathematical Institute, University of Oxford, UK, host: Prof. Xiaowen Dong.
  - 02/2023 Department of Computer Science, Texas A&M University, USA, host: Prof. Shuiwang Ji.
  - Centre for Frontier AI Research, A*STAR, Singapore, host: Dr. Ivor Tsang, Prof. Ong Yew-Soon.
  - Amazon Research, USA, host: Aishwarya Reganti.
  - 01/2023 Prescient Design, Genentech, Roche, Switzerland/USA, host: Dr. Andreas Loukas.
  - 12/2022 NeurIPS 2022 Workshop on Symmetry and Geometry, New Orleans, USA, oral presentation.
  - 10/2022 Department of Computer Science, NUS, Singapore, host: Prof. Bryan Hooi.
  - Institute for Infocomm Research, A*STAR, Singapore, host: Prof. Xiaoli Li.

Publications

Equal first authorship/contribution is indicated using †, and highlighted works are indicated using ★. Latest publication list and citations can be found on my Google Scholar profile (2.7K+ citations).

Preprints

2023

1. A. Duval†, S. V. Mathis†, **C. K. Joshi**†, V. Schmidt†, S. Miret, F. D. Malliaros, T. Cohen, P. Lio, Y. Bengio, and M. Bronstein: *A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems*, 2023. Materials are used in courses at Stanford (CS224W), Cambridge (L65), Oxford (GDL), etc. arXiv: 2312.07511 ★
2. X. Zhang, L. Wang, J. Helwig, …, **C. K. Joshi**, …, T. Smidt, and S. Ji: *Artificial intelligence for science in quantum, atomistic, and continuum systems*, 2023. 62 authors, 263 pages survey on AI4Science led by Prof. Shuiwang Ji, I contributed to *Molecular Representation Learning* section. arXiv: 2307.08423

Conference publications

2025

3. **C. K. Joshi**, A. R. Jamasb, R. Viñas, C. Harris, S. Mathis, A. Morehead, R. Anand, and P. Liò: *gRNAde: Geometric Deep Learning for 3D RNA inverse design*. International Conference on Learning Representations (ICLR), 2025. Also **Spotlight presentation** at MLCB 2024. arXiv: 2305.14749 ★

2024

4. R. Anand†, **C. K. Joshi**†, A. Morehead, A. R. Jamasb, C. Harris, S. Mathis, K. Didi, B. Hooi, and P. Liò: *RNA-FrameFlow: Flow Matching for de novo 3D RNA backbone design*. Machine Learning for Computational Biology (MLCB), 2024. **Oral presentation**. Also **Oral presentation** at ICML 2024 Workshops on Structured Generative Modeling as well as AI4Science. arXiv: 2406.13839
5. A. R. Jamasb†, A. Morehead†, **C. K. Joshi**†, Z. Zhang†, K. Didi, S. V. Mathis, C. Harris, J. Tang, J. Cheng, P. Liò, and T. L. Blundell: *Evaluating Representation Learning on the Protein Structure Universe*. International Conference on Learning Representations (ICLR), 2024. arXiv: 2406.13864

2023

6. **C. K. Joshi**†, C. Bodnar†, S. V. Mathis, T. Cohen, and P. Liò: *On the Expressive Power of Geometric Graph Neural Networks*. International Conference on Machine Learning (ICML), 2023. Also **Oral presentation** at NeurIPS 2022 Workshop of Symmetry & Geometry. arXiv: 2301.09308 ★

2022 7. F. Liu, G. Lin, C.-S. Foo, **C. K. Joshi**, and J. Lin: *Point Discriminative Learning for Unsupervised Representation Learning on 3D Point Clouds*. International Conference on 3D Computer Vision (3DV), 2022. arXiv: 2108.0210

2021 8. **C. K. Joshi**, Q. Cappart, L.-M. Rousseau, and T. Laurent: *Learning TSP Requires Rethinking Generalization*. International Conference on Principles and Practice of Constraint Programming, 2021. arXiv: 2006.07054

Journal publications

2023 9. R. Viñas, **C. K. Joshi**, D. Georgiev, B. Dumitrascu, E. R. Gamazon, and P. Liò: *Hypergraph Factorisation for Multi-tissue Gene Expression Imputation*. Nature Machine Intelligence 5:7, pp. 739–753, 2023. **Cover article**. DOI: 10.1038/s42256-023-00684-8

10. V. P. Dwivedi, **C. K. Joshi**, T. Laurent, Y. Bengio, and X. Bresson: *Benchmarking Graph Neural Networks*. Journal of Machine Learning Research 24:43, pp. 1–48, 2023. **2.5K+ stars on GitHub**. arXiv: 2003.00982 ★

2022 11. **C. K. Joshi**, F. Liu, X. Xun, J. Lin, and C.-S. Foo: *On Representation Knowledge Distillation for Graph Neural Networks*. IEEE Transactions of Neural Networks and Learning Systems, 2022. DOI: 10.1109/TNNLS.2022.3223018. arXiv: 2111.04964

12. **C. K. Joshi**, Q. Cappart, L.-M. Rousseau, and T. Laurent: *Learning the Travelling Salesperson Problem Requires Rethinking Generalization*. Constraints, pp. 1–29, 2022. **Invited article**. DOI: 10.1007/s10601-022-09327-y. arXiv: 2006.07054

2021 13. P. Xu, **C. K. Joshi**, and X. Bresson: *Multi-Graph Transformer for Free-Hand Sketch Recognition*. IEEE Transactions of Neural Networks and Learning Systems, 2021. DOI: 10.1109/TNNLS.2021.3069230. arXiv: 1912.11258

Book chapters

2024 14. **C. K. Joshi** and P. Liò: *gRNAde: A Geometric Deep Learning Pipeline for 3D RNA Inverse Design*. RNA Design: Methods and Protocols. **Invited book chapter**, pp. 121–135, Springer, Methods in Molecular Biology (MIMB, volume 2847), 2024.

Patents

2020 15. S. Saito, T. V. Le, **C. K. Joshi**, and R. Shanmugamani: *Representing Sets of Entitites for Matching Problems*. US Patent App. 16/208,681.

16. S. Saito, **C. K. Joshi**, R. Shanmugamani, T. V. Le, and R. Arumugam: *Utilizing Embeddings for Efficient Matching of Entities*. US Patent App. 16/217,148.

17. T. V. Le, S. Saito, **C. K. Joshi**, and R. Shanmugamani: *Graphical Approach to Multi-Matching*. US Patent App. 16/210,070.

Workshop papers and informal publications

2023 18. C. Harris, K. Didi, A. R. Jamasb, **C. K. Joshi**, S. V. Mathis, P. Lio, and T. Blundell: *PoseCheck: Generative Models for 3D Structure-based Drug Design Produce Unrealistic Poses*. NeurIPS Workshop on Machine Learning for Structural Biology, 2023. arXiv: 2308.07413

19. K. Bujel[†], Y. Gideoni[†], **C. K. Joshi**, and P. Liò: *Group Invariant Global Pooling*. ICML Workshop on Topology, Algebra, & Geometry, 2023. arXiv: 2305.19207

2020 20. **C. K. Joshi**: *Transformers are Graph Neural Networks*. The Gradient. **Read 100,000+ times**, featured in *Probabilistic ML textbook* by Kevin Murphy, taught in courses at Stanford (CS224W), Cambridge (L45), Oxford (GDL), etc. URL. 2020. ★

2019 21. **C. K. Joshi**, T. Laurent, and X. Bresson: *An Efficient Graph Convolutional Network Technique for the Travelling Salesman Problem*. INFORMS Annual Meeting, Session on Boosting Combinatorial Optimization using Machine Learning, 2019. arXiv: 1906.01227

Open Source Software

All my code is available on my GitHub (5K+ total stars).

150+ stars
- **Geometric RNA Design (gRNAde)**: A toolkit for generative 3D RNA inverse design (ICLR 2025).

200+ stars
- **ProteinWorkshop**: A benchmarking framework for deep learning on 3D protein structure (ICLR 2024).

450+ stars
- **Geometric GNN Dojo**: Pedagogical implementations and experiments on 3D GNNs (ICML 2023).

2,500+ stars
- **Benchmarking GNNs**: A benchmarking framework for Graph Neural Networks (JMLR 2023).

Teaching experience

I have served as a teaching assistant/supervisor for the following courses.

2022, 2023, 2024
- **Representation Learning on Graphs**, M.Phil. in Advanced Computer Science, University of Cambridge, UK; instructors: Prof. Pietro Liò, Dr. Petar Veličković (Google DeepMind).
  Lead the creation & grading of practical sessions on *Geometric Graph Neural Networks* (100+ students). Delivered guest lectures on *Introduction to Graph Generative Models* (2023) and *Geometric Graph Neural Networks* (2024). Supervised term project for 17 students.

2022, 2023
- **Introduction to Artificial Intelligence**, Part IB in Computer Science, University of Cambridge, UK; instructor: Prof. Sean Holden.
  Developed personalised supervision sessions for 12 undergraduate students.

Mentorship & Supervision

2024
- Batu El, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
  Term project: *Mechanistic Interpretability of Graph Neural Networks and Transformer*.
  Next: Ph.D. Student, Stanford University, USA. **Knight-Hennessey Scholar**.
- Deepro Chaudhury, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
  Term project: *Mechanistic Interpretability of Graph Neural Networks and Transformer*.
  Next: Ph.D. Student, University of Oxford, UK; supervisor: Prof. Tom Rainforth.
- Vladimir Radenkovic, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
  MPhil thesis: *Molecular Dynamics-conditioned Protein Design with SE(3) Flow Matching*.
  Next: Ph.D. Student, University of Cambridge, UK; supervisor: Prof. Tuomas Knowles, Prof. Pietro Liò.
- Rishabh Anand, B.Sc. in Computer Science, National University of Singapore.
  Bachelor's thesis: *Generative Modelling for 3D RNA Structure Design*.
  Next: M.Sc. Student, Yale University, USA; advisors: Prof. Smita Krishnaswamy, Prof. Rex Ying.
  Outstanding Undergraduate Researcher Award, Best Poster Award.

2023
- Yonatan Gideoni, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
  Term project: *Group Invariant Global Pooling*.
  Next: Ph.D. Student, University of Oxford, UK; supervisors: Prof. Yarin Gal, Prof. Michael Bronstein.
  Rhodes Scholar.
- Teodora Reu, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
  MPhil thesis: *Reimagining Graph Topology: Exploring Variational and Attentional Approaches*.
  Next: Ph.D. Student, University of Oxford, UK; supervisor: Prof. Michael Bronstein.
- Kamil Bujel, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
  MPhil thesis: *Learning and Breaking Symmetries in Geometric Deep Learning*.
  Next: Quant Researcher, Jump Trading, London, UK.
- Harry Shaw, Part III in Physics, Unversity of Cambridge, UK.
  MPhil thesis: *Expressive Equivariant Graph Neural Networks with Higher Rank Cartesian Tensors*.
  Next: Quant Researcher, Citadel, London, UK.

2022
- Peter Ralbovsky, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
  Term project: *Geometrically Equivariant GNNs for Travelling Salesman Problem*.
  Next: Software Engineer, Google, Zurich, Switzerland.

Academic Service

Organisation

04/2025 • **Organiser, ICLR 2025 Workshop on Artificial Intelligence for Nucleic Acids**

2022, 2023, 2024 • **General Chair & Organiser, Learning on Graphs Conference**
LoG is a new annual research conference for machine learning on graphs and geometry founded by professors, scientists, and PhD students from Cambridge, Oxford, Stanford, MIT, Google DeepMind, etc. LoG emphasizes on review quality through a curated program committee and monetary rewards for top reviewers. LoG also aims to build an inclusive and global community by being fully virtual and free to attend, as well as supporting local mini-conferences around the world. As General Chair in 2024, I lead a team of 24 on all aspects of the conference, including handling 200+ submissions, 35K+ USD in sponsorship, and 15+ local meetups across USA, Europe, China, and India.

06/2023 • **Organiser, Understanding Biology in the age of Artificial Intelligence**
Conference in Cambridge exploring AI in biology from three perspectives: *theory*, *science*, and *philosophy*. Awarded GBP 14,000 grant from Accelerate Science and Cambridge Centre for Data-Driven Discovery. Keynote speakers included Pushmeet Kohli (Google DeepMind), Charlotte Deane (University of Oxford), and Sarah Teichmann (Sanger Institute).

Reviewing

- *Conferences*

International Conference on Machine Learning (ICML)	2022–2025
Advances in Neural Information Processing Systems (NeurIPS)	2021–2024
International Conference on Learning Representations (ICLR)	2022–2024

- *Journals*

IEEE Transactions on Pattern Analysis & Machine Intelligence (TPAMI)	2022
IEEE Transactions on Neural Networks & Learning Systems (TNNLS)	2022
Distill	2021

Press coverage

07/2024 • "Qualcomm Innovation Fellowship Europe Rewards Excellent Research in the Field of AI and Cybersecurity", Qualcomm Inc.

• PhD student awarded Qualcomm Innovation Fellowship, Department of Computer Science, University of Cambridge.

03/2024 • "The rise of Dawn: How the UK's fastest AI supercomputer is supporting goals in clean energy, personalised medicine and climate.", University of Cambridge covering the launch of selected pilot projects for *Dawn*, the UK's new AI supercomputer based in Cambridge, including my work on *Geometric Deep Learning for RNA Design*.

08/2023 • "New computational method can integrate gene expression across multiple tissue types", Department of Computer Science, University of Cambridge announcing our cover article in *Nature Machine Intelligence*.

11/2022 • "Clare Hall students win prestigious 14K GBP grant", Clare Hall, University of Cambridge announcing our grant to organise a conference titled *Understanding Biology in the Age of AI*.

03/2021 • "Stars in the making", A*STAR Research Magazine.

03/2020 • "Yoshua Bengio and team introduce GNN benchmarking framework", Synced Review Magazine.

08/2019 • "The path behind, the road ahead", NTU Class of 2019 Valedictorians, NTULink Alumni Magazine.