Sékou-Oumar Kaba

Curriculum Vitae

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Research interests: AI for science, Geometric deep learning, Generative models, Materials physics

Education

Doctor of Philosophy in Computer Science GPA: 3.9/4.0 — 2020 – 2025
McGill University
Supervisor: Prof. Siamak Ravanbakhsh
Equivariant neural networks for predictive and generative models.

Master of Science in Physics GPA: 4.1/4.3 — 2016 – 2018
Université de Sherbrooke
Supervisor: Prof. David Sénéchal
Symmetry of the order parameter in multi-orbital superconductors with quantum cluster methods.

Bachelor of Science in Physics — 2013 – 2016
Université Laval

Employment

Research-related

Research Intern in Machine Learning — 2023
Microsoft Research Amsterdam
Supervisor: Dr. Giulia Luise
Deep learning for quantum chemistry and electronic structure.

Research Intern in Machine Learning — 2019 – 2020
Mila - Quebec Artificial Intelligence Institute
Supervisor: Prof. Yoshua Bengio
Deep learning models for material property prediction and identification of candidates for magnetic refrigeration.

Research Intern in Neuroscience — 2015
CERVO Brain Research Center
Supervisor: Prof. Robert Bonin
Optogenetics and behavioural experiments on mice. Segmentation algorithms for cell microscope imaging.

Industry-related

Scientific Developer — 2018 – 2019
OODA Technologies
Full-stack development of data analysis software, with applications in geolocation, NLP and computer vision.

Data Scientist — 2018 – 2019
The Brane
Data scraping and processing from scientific databases to populate knowledge graphs.

Awards and grants

Scholarships (total funding: 238,800$)

- FRQNT Doctoral Training Scholarship (25 000$/year) — 2023 – 2025
- DeepMind PhD Scholarship (13 600$/year) — 2021 – 2024
- IVADO PhD Excellence Scholarship (25 000$/year) — 2021 – 2024
- McGill Departmental Award (6 000$/year) — 2021 – 2025
- DeepMind Masters Scholarship (12 000$/year) — 2020 – 2021

Grants

I made significant contributions to writing the following grant proposal during my Ph.D. :

- Samsung SAIT Call for Projects (60 000$) 2022
  PIs : Siamak Ravanbakhsh and Yoshua Bengio; Industrial partner : Yan Zhang

Awards

- Laureate of the Acfas national science popularization contest (Press coverage) 2018
- Best oral presentation award, CGCQC 2018

Publications

Conference papers

- X. Li, **S.-O. Kaba**, S. Ravanbakhsh. 2025
  On the identifiability of causal abstractions
  Under review at the International Conference on Artificial Intelligence and Statistics (AISTATS)
- D. Levy*, S. Panigrahi*, **S.-O. Kaba***, Q. Zhu, K. Lee, M. Galkin, S. Miret, S. Ravanbakhsh. 2025
  SymmCD: Symmetry-preserving crystal generation with diffusion models
  Under review at the International Conference on Learning Representations (ICLR)
- H. Lawrence, V. Portilheiro, Y. Zhang, **S.-O. Kaba**. 2025
  Improving equivariant networks with probabilistic symmetry breaking
  Under review at the International Conference on Learning Representations (ICLR)
- A. K. Mondal, S. Panigrahi, **S.-O. Kaba**, S. Rajeswar, S. Ravanbakhsh. 2023
  Equivariant adaptation of large pre-trained models
  Conference on Neural Information Processing Systems (NeurIPS)
- **S.-O. Kaba***, A. K. Mondal*, Y. Zhang, Y. Bengio, S. Ravanbakhsh. 2023
  Equivariance with learned canonicalization functions
  International Conference on Machine Learning (ICML)
- **S.-O. Kaba**, S. Ravabakhsh. 2022
  Equivariant networks for crystal structures
  Conference on Neural Information Processing Systems (NeurIPS)
- M. Pezeshki, **S.-O. Kaba**, Y. Bengio, A. Courville, D. Precup, and G. Lajoie. 2021
  Gradient starvation: A learning proclivity in neural networks
  Conference on Neural Information Processing Systems (NeurIPS)

Journal articles

- **S.-O. Kaba**, B. Groleau-Paré, M.-A. Gauthier, A.-M. S. Tremblay, S. Verret, and C. Gauvin-Ndiaye. 2023
  Prediction of large magnetic moment materials with graph neural networks and random forests
  Physical Review Materials
- **S.-O. Kaba** and D. Sénéchal. 2019
  Group-theoretical classification of superconducting states of strontium ruthenate
  Physical Review B

Peer-reviewed workshop papers

- D. Levy*, S. Panigrahi*, **S.-O. Kaba***, Q. Zhu, K. Lee, M. Galkin, S. Miret, S. Ravanbakhsh. 2024
  SymmCD: Symmetry-preserving crystal generation with diffusion models
  NeurIPS Workshop on AI for Accelerated Materials Design (AI4Mat)
  Oral, top 20% of accepted submissions

*Denotes equal contribution

- H. Lawrence, V. Portilheiro, Y. Zhang, **S.-O. Kaba**. 2024
  Improving equivariant networks with probabilistic symmetry breaking
  ICML Workshop on Geometry-grounded Representation Learning and Generative Modeling (GRaM)
- **S.-O. Kaba**, S. Ravanbakhsh. 2023
  Symmetry breaking and equivariant neural networks
  NeurIPS Workshop on Symmetry and Geometry in Neural Representations (NeurReps)
  Oral, top 20% of accepted submissions
- D. Levy*, **S.-O. Kaba***, C. Gonzales, S. Miret, S. Ravanbakhsh. 2023
  Using multiple vector channels improves E(n)-equivariant graph neural networks
  ICML Workshop on Machine Learning for Astrophysics
- **S.-O. Kaba***, A. K. Mondal*, Y. Zhang, Y. Bengio, S. Ravanbakhsh. 2022
  Equivariance with learned canonicalization functions
  NeurIPS Workshop on Symmetry and Geometry in Neural Representations (NeurReps)
  Oral, top 15% of accepted submissions

Selected presentations

- *Generative models for materials*. Université de Montréal, Physics Department 2024
- *Breaking symmetries with equivariant neural networks and GNNs*. Learning on Graphs Conference 2024
- *Advances in deep learning for materials discovery*. IBM Quantum 2024
- *AI for materials discovery*. Deep Learning IndabaX Cameroon (**Keynote**) 2024
- *AI for materials discovery*. Mila Quantum and AI Day (**Keynote**) 2024
- *Valoriser les communautés noires en IA*. IVADO (**Panel**) 2024
- *Equivariance with learned canonicalization functions*. Ciela Institute 2023
- *Equivariant networks for crystal structures*. Learning on Graphs Conference 2022
- *Zoom sur la recherche en physique de la matière condensée*. SAPHARI Symposium 2019
- *Superconductivity in Sr_2RuO_4 with quantum cluster methods*. CGQC (**Best Presentation Award**) 2018

Technical skills and software

Programming: Python, Java, JavaScript **Environment**: Mac OS, Linux, Windows

Technologies: Pytorch, SciPy, HuggingFace, Git, LaTeX, Docker, MongoDB, SQL, React, Spring

Open source software contributions

- EquiAdapt: Equivariant adaptation of neural networks (documentation)
- Equivariant networks for crystal structures (code)

Teaching and supervision

Teaching assistant

- COMP 588: Probabilistic Graphical Models, McGill University 2024
- PHQ 344: Statistical Mechanics I, Université de Sherbrooke 2017
  Implemented an active learning approach and taught workshops 1 hour/week

Internship co-supervisor

- Jikael Gagnon, McGill University 2024
- Jonathan Clepkens, Université de Sherbrooke 2018

Professional service

Event Organization

Workshop Organizer and Program Chair 2024
ICML 2024 Workshop on Geometry-grounded Representation Learning and Generative Modeling (GRaM)

Reading Group Organizer 2023 – 2024
Mila's Geometric Deep Learning Reading Group

Workshop Organizer 2023
Mila Quantum and AI day

Communications and Media Coordinator 2018
Women in Physics Canada Conference

Reviewing

- International Conference on Learning Representations (ICLR) 2025
- International Conference on Artificial Intelligence (AAAI) 2025
- SciPost Physics 2024
- Learning on Graphs Conference 2024
- NeurIPS Workshop on Symmetry and Geometry in Neural Representations 2024
- NeurIPS Workshop on AI for Accelerated Materials Design 2024
- Transactions on Machine Learning Research (TMLR) 2024
- International Conference on Machine Learning (ICML) 2024
- Nature Machine Intelligence 2024
- Conference on Neural Information Processing Systems (NeurIPS) 2023
- Science Advances 2023
- NeurIPS Workshop on Topology, Algebra and Geometry in Machine Learning 2023

Outreach

Science Communication Consultant 2019 – 2024
Association canadienne francophone pour le savoir (Acfas)

Student Mentor 2020 – 2021
Projet SEUR

Radio Host 2018
CISM and CFAK
Co-hosted the weekly radio show Aujourd'hui, c'est déjà demain, aired on two radio stations and as a podcast.

Technical Director 2015 – 2016
Coupe de Science

Science Popularizer 2015
Boite à Science

Leadership positions

Laboratory Representative 2020 – 2022
Mila - Quebec Artificial Intelligence Institute

Vice President External 2017 – 2018
Regroupement étudiant des chercheurs en sciences de l'Université de Sherbrooke

Vice President Academic 2015 – 2016
Association des étudiants de physique de l'Université Laval