Sékou-Oumar Kaba

Curriculum Vitae

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Research interests: AI for science, Geometric deep learning, Generative models, Solid-state 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: 283,400$)

- FRQNT Doctoral Training Scholarship (75 000$) — 2023 – 2025
- DeepMind PhD Scholarship (54 400$) — 2021 – 2024
- IVADO PhD Excellence Scholarship (100 000$) — 2021 – 2024
- McGill Departmental Award (30 000$) — 2021 – 2025
- DeepMind Masters Scholarship (24 000$) — 2020 – 2021

Grants

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

- Samsung SAIT Call for Projects (80 000$) 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

- **S.-O. Kaba***, K. Sareen*, D. Levy, S. Ravanbakhsh. 2025
  Energy loss functions for physical systems
  Under review at the Conference on Neural Information Processing Systems (NeurIPS)
- H. Lawrence, V. Portilheiro, Y. Zhang, **S.-O. Kaba**. 2025
  Improving equivariant networks with probabilistic symmetry breaking
  International Conference on Learning Representations (ICLR)
- 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
  International Conference on Learning Representations (ICLR)
- X. Li, **S.-O. Kaba**, S. Ravanbakhsh. 2025
  On the identifiability of causal abstractions
  International Conference on Artificial Intelligence and Statistics (AISTATS)
- 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

- K. Sareen, D. Levy, A. K. Mondal, **S.-O. Kaba**, T. Akhound-Sadegh, S. Ravanbakhsh. 2024
  Symmetry-aware generative modeling through learned canonicalization
  NeurIPS Workshop on Symmetry and Geometry in Neural Representations (NeurReps)
- 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

Preprints

- G. Luise *et al.* (**S.-O. Kaba included**) 2025
  Accurate and scalable exchange-correlation with deep learning

Open source software contributions

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

Selected presentations

Invited talks

- *Energy loss functions for physical systems*. Samsung AI, Korea 2025
- *Equivariance, symmetry breaking and positional encodings*. KAIST-Mila Prefrontal Center 2025
- *Improving equivariant networks with probabilistic symmetry breaking*. Samsung SAIT, Montreal, Canada 2025
- *Generative models for materials*. Université de Montréal, Physics Department, Montreal, Canada 2024
- *Advances in deep learning for materials discovery*. IBM Quantum, Sherbrooke, Canada 2024
- *AI for materials discovery*. Deep Learning IndabaX, Yaounde, Cameroon (**Keynote**) 2024
- *AI for materials discovery*. Mila Quantum and AI Day, Montreal, Canada 2024
- *Valoriser les communautés noires en IA*. IVADO, Montreal, Canada (**Panel**) 2024
- *Zoom sur la recherche en physique de la matière condensée*. SAPHARI Symposium, Montreal, Canada 2019

Contributed talks

- *Breaking symmetries with equivariant neural networks*. Learning on Graphs Conference, Montreal, Canada 2024
- *Symmetry breaking and equivariant neural networks*. NeurIPS NeurReps Workshop, New Orleans, USA 2023
- *Equivariance with learned canonicalization functions*. NeurIPS NeurReps Workshop, New Orleans, USA 2022
- *Equivariant networks for crystal structures*. Learning on Graphs Conference, Montreal, Canada 2022
- *Superconductivity in Sr_2RuO_4 with quantum cluster methods*. CGQC, Vancouver, Canada 2018
  (**Best Presentation Award**)

Teaching and supervision

Guest Lecturer

- COMP 511: Network Science, *Expressivity of graph neural networks*, McGill University 2025

Teaching assistant

- COMP 588: Probabilistic Graphical Models, McGill University 2025
  Contributed to desinging assignments and graded
- PHQ 344: Statistical Mechanics I, Université de Sherbrooke 2017
  Implemented an active learning approach, taught workshops 1 hour/week and graded

Internship co-supervisor

- Jikael Gagnon, McGill University 2024
  Project: Quantum hamiltonians for equivariant molecular deep learning.
- Xiusi Li, McGill University 2023
  Project: Identifiability of causal models and abstractions.
- Jonathan Clepkens, Université de Sherbrooke 2018
  Project: Variational cluster approximation for superconductivity in strontium ruthenate.

Professional service

Event Organization

Workshop Organizer and Program Chair 2024
ICML 2024 Workshop on Geometry-grounded Representation Learning and Generative Modeling (GRaM)
Coordinated the scientific program, review process and organization of a workshop at ICML.
147 works were accepted and 11 talks presented.

Reading Group Organizer 2023 – 2024
Mila's Geometric Deep Learning Reading Group
Led the organization and scientific program of a weekly reading group on geometric deep learning.

Workshop Organizer 2023
Mila Quantum and AI Day
Organized a workshop bringing together academic and industry experts on the intersection between AI and quantum sciences.

Communications and Media Coordinator 2018
Women in Physics Canada Conference
Managed outreach, content creation, and communications for a national conference advancing gender diversity in physics.

Outreach

Science Communication Consultant 2019 – 2024
Association canadienne francophone pour le savoir (Acfas)
Provided expert feedback to researchers on improving the clarity and impact of their science communication.
Served as a judge for national science popularization contests.

Student Mentor 2020 – 2021
Projet SEUR
Mentored 4 high school students on research projects to encourage continuation of studies.

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

Technical Director 2015 – 2016
Coupe de Science
Managed the technical operations of a science competition for 100+ high school students.

Science Popularizer 2015
Boîte à Science
Led hands-on science outreach activities for youth to promote curiosity and engagement in STEM.

Leadership positions

Steering Committee Memeber 2025
Mila - Quebec Artificial Intelligence Institute
Student representative on the steering committee charged to support strategic planning and institutional restructuring.

Laboratory Representative 2020 – 2022
Mila - Quebec Artificial Intelligence Institute
Acted as a representative for graduate students with institute leadership.

Vice President External 2017 – 2018
Regroupement étudiant des chercheurs en sciences de l'Université de Sherbrooke (RECSUS)
Represented graduate student interests in scientific research policy and external affairs.

Vice President Academic 2015 – 2016
Association des étudiants de physique de l'Université Laval (ADEPUL)
Advocated for students on academic policies and organized initiatives to support physics education.

Reviewing

Conferences

- International Conference on Machine Learning (ICML) 2024, 2025
- International Conference on Learning Representations (ICLR) 2025
  - ICLR Workshop on Frontiers in Probabilistic Inference 2025
  - ICLR Workshop on AI for Accelerated Materials Design 2025
- Conference on Neural Information Processing Systems (NeurIPS) 2023, 2025
  - NeurIPS Workshop on Symmetry and Geometry in Neural Representations 2022 – 2024
  - NeurIPS Workshop on AI for Accelerated Materials Design 2022 – 2024
  - NeurIPS Workshop on Topology, Algebra and Geometry in Machine Learning 2023
- International Conference on Artificial Intelligence (AAAI) 2025
- Learning on Graphs Conference 2024

Journals

- Nature Communications 2025
- SciPost Physics 2025
- Transactions on Machine Learning Research (TMLR) 2024
- Nature Machine Intelligence 2023, 2024
- Science Advances 2023