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

Preprints

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

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*Denotes equal contribution

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

- 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

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

- *Accurate and scalable exchange-correlation with deep learning.* RQÉMP Summer School, Sherbrooke, Canada   2025
- *Symmetry-preserving crystal generation with diffusion models.* SIAM Annual Meeting, Montreal, Canada   2025
- *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

Lecturer
- COMP 551: Applied Machine Learning, 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

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

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