

# 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

- 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. Ravanbakhsh. 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*

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\*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

<b>Workshop Organizer and Program Chair</b>	2024
ICML 2024 Workshop on Geometry-grounded Representation Learning and Generative Modeling (GRaM)	
<b>Reading Group Organizer</b>	2023 – 2024
Mila's Geometric Deep Learning Reading Group	
<b>Workshop Organizer</b>	2023
Mila Quantum and AI day	
<b>Communications and Media Coordinator</b>	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

<b>Science Communication Consultant</b>	2019 – 2024
Association canadienne francophone pour le savoir (Acfas)	
<b>Student Mentor</b>	2020 – 2021
Projet SEUR	
<b>Radio Host</b>	2018
CISM and CFAK	
<i>Co-hosted the weekly radio show Aujourd'hui, c'est déjà demain, aired on two radio stations and as a podcast.</i>	
<b>Technical Director</b>	2015 – 2016
Coupe de Science	
<b>Science Popularizer</b>	2015
Boite à Science	

### Leadership positions

<b>Laboratory Representative</b>	2020 – 2022
Mila - Quebec Artificial Intelligence Institute	
<b>Vice President External</b>	2017 – 2018
Regroupement étudiant des chercheurs en sciences de l'Université de Sherbrooke	
<b>Vice President Academic</b>	2015 – 2016
Association des étudiants de physique de l'Université Laval	