# Sékou-Oumar Kaba

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Machine learning Ph.D. student with a physics background and data science industry experience. My interests include **AI** for science, **Geometric Deep Learning**, **Graph Representation Learning**.

## **Education**

## **Doctor of Philosophy in Computer Science**

Montréal

McGill University

Since 2020

GPA: 3.9 / 4.0

Supervisor: Prof. Siamak Ravanbakhsh

Designing deep learning models that leverage symmetry in materials for prediction and generation.

## Master of Science in Physics

Université de Sherbrooke

Sherbrooke

2016 - 2018

GPA: 4.1 / 4.3

Supervisor: Prof. David Sénéchal

Conducted numerical simulations on quantum lattice models to study unconventional superconductivity.

#### **Bachelor of Science in Physics**

Québec

Université Laval 2013 - 2016

## Research experience

#### Research Intern in AI for Science

**Amsterdam** 

Microsoft Research Amsterdam Supervisor: Dr. Giulia Luise

Research Intern in Machine Learning

Montréal

2023

Mila - Quebec Artificial Intelligence Institute

2019 - 2020

Supervisor: Prof. Yoshua Bengio

 Implemented deep learning models for material property prediction. Performed predictions on a database of existing materials to identify promising candidates for magnetic refrigeration.

#### Research Intern in Neuroscience

Québec

CERVO Brain Research Center (Formerly CRIUSMQ)

2015

Supervisor: Prof. Robert Bonin

 Designed and performed optogenetics and behavioural experiments on mice to study the MrgprB4 expressing neurons suspected to play a role in chronic pain.

# **Industry experience**

## Scientific Developer

Montréal

OODA Technologies

2018 - 2019

• Full-stack work on data collection, analysis, and visualization programs, with applications in geolocation and computer vision. Tested, debugged, and documented software products.

Data Scientist Montréal

The Brane 2018 - 2019

Scraped and processed data from various scientific databases to populate knowledge graphs. Engineered ontologies for the extracted data.

## **Publications**

#### Conference papers:

- A. K. Mondal, S. S. Panigrahi, **S.-O. Kaba**, S. Rajeswar, S. Ravanbakhsh. *Equivariant adaptation of large pre-trained models*, Advances on Neural Information Processing Systems 36 (NeurIPS), 2023.
- **S.-O. Kaba\***, A. K. Mondal\*, Y. Zhang, Y. Bengio, S. Ravanbakhsh. *Equivariance with learned canonicalization functions.*, International Conference on Machine Learning (ICML), 2023.
- **S.-O. Kaba**, S. Ravabakhsh. *Equivariant networks for crystal structures*. Advances on Neural Information Processing Systems 35 (NeurIPS), 2022.
- M. Pezeshki, **S.-O. Kaba**, Y. Bengio, A. Courville, D. Precup, and G. Lajoie. *Gradient starvation: A learning proclivity in neural networks*. Advances on Neural Information Processing Systems 34 (NeurIPS), 2021.

#### Workshop papers:

- **S.-O. Kaba**, S. Ravanbakhsh. *Symmetry breaking and equivariant neural networks.* NeurIPS 2023 Workshop on Symmetry and Geometry in Neural Representations, 2023. **(Oral)**
- **S.-O. Kaba\***, A. K. Mondal\*, Y. Zhang, Y. Bengio, S. Ravanbakhsh. *Equivariance with learned canonicalization functions*. NeurIPS 2022 Workshop on Symmetry and Geometry in Neural Representations, 2022. (**Spotlight**)
- D. Levy\*, **S.-O.** Kaba\*, C. Gonzales, S. Miret, S. Ravanbakhsh. *Using multiple vector channels improves* E(n)-equivariant graph neural networks. ICML Workshop on Machine Learning for Astrophysics, 2023.

#### Journal articles:

- **S.-O. Kaba**, B. Groleau-Paré, M.-A. Gauthier, A.-M. S. Tremblay, S. Verret, and C. Gauvin-Ndiaye. *Prediction of large magnetic moment materials with graph neural networks and random forests.* Phys. Rev. Mater., 7:044407, 2023.
- **S.-O. Kaba** and D. Sénéchal. *Group-theoretical classification of superconducting states of strontium ruthenate*. Phys. Rev. B, 100:214507, 2019.

#### Presentations:

Equivariant networks for crystal structures. Learning on Graphs Conference, Montréal, Canada, 2022. Superconductivity in strontium ruthenate with quantum cluster methods. Canadian Graduate Quantum Conference, Vancouver, Canada, 2018. (Best presentation award)

#### Invited talks and panels:

Valoriser les communautés noires en IA. IVADO, Canada, 2022.

Zoom sur la recherche en physique de la matière condensée. SAPHARI Symposium, Montréal, Canada, 2019.

## **Summer schools**

o CIFAR Deep Learning and Reinforcement Learning Summer School, Canada	2022
o International Physics School on Quantum Materials, Sherbrooke, Canada	2017

#### Awards and achievements

## Scholarships:

FRQNT Doctoral Training Scholarship (25 000\$)	2023 - 2025
DeepMind PhD Scholarship (13 600\$)	2021 - 2024
IVADO PhD Excellence Scholarship (25 000\$)	2021 - 2024
DeepMind Masters Scholarship (12 000\$)	2020 - 2021

#### Awards:

Samsung SAIT Call for Projects, Pls: Siamak Ravanbakhsh and Yoshua Bengio (60 000\$)

## **Technical skills**

Technologies: Pytorch, Git, LATEX, Docker, MongoDB, ArangoDB, React, Spring, Flask

## Other experience

# Academic

#### Reviewer

- Advances on Neural Information Processing Systems (NeurIPS)
- Science Advances
- Nature Machine Intelligence
- NeurIPS Workshop on Symmetry and Geometry in Neural Representations (NeurReps)
- o ICML Workshop on Topology, Algebra and Geometry in Machine Learning (TAG-ML)
- NeurIPS Workshop on AI for Accelerated Materials Design (AI4Mat)

Reading Group Organizer	Montréal
Co-organized the Geometric Deep Learning Reading Group at Mila	Since 2023
Workshop Organizer Co-organized the Quantum and Al Day at Mila	<b>Montréal</b> 2023
Teaching	

Teaching Assistant
Université de Sherbrooke

Sherbrooke
2017

Course: Statistical Mechanics I

Prepared and taught weekly tutorial sessions using an active learning approach

Science InstructorQuébecCégep de Sainte-Foy2013 - 2015

## Outreach

Science Communication Consultant

Acfas

Montréal

Since 2019

Radio Host Montréal

CISM (Montréal) and CFAK (Sherbrooke)

2018

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

Science Popularizer

Québec

Boîte à science

2014

## Community service

Laboratory RepresentativeMontréalMila - Quebec Artificial Intelligence Institute2020 - 2022

**Student Mentor**Projet SEUR
2019 - 2021

Vice President External Sherbrooke

Regroupement étudiant des chercheurs en sciences de l'Université de Sherbrooke 2017 - 2018

Vice President Academic Québec

Association des étudiants de physique de l'Université Laval 2015 - 2016