Sékou-Oumar Kaba

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Education

Doctor of Philosophy in Computer Science (GPA : 3.9 / 4.0)
McGill University *2020 - 2025*
Supervisor: Prof. Siamak Ravanbakhsh
- Designing deep learning models that leverage symmetry for prediction and generation tasks.

Master of Science in Physics (GPA : 4.1 / 4.3)
Université de Sherbrooke *2016 - 2018*
Supervisor: Prof. David Sénéchal
- Conducted numerical simulations on quantum lattice models to study unconventional superconductivity.

Bachelor of Science in Physics
Université Laval *2013 - 2016*

Employement

Research-related

Research Intern in AI for Science
Microsoft Research Amsterdam *2023*
Supervisor: Dr. Giulia Luise
- Worked on machine learning for quantum chemistry.

Research Intern in Machine Learning
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
CERVO Brain Research Center *2015*
Supervisor: Prof. Robert Bonin
- Designed and performed optogenetics and behavioural experiments on mice and implemented a segmentation algorithm for cell microscope imaging.

Industry-related

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

Data Scientist
The Brane *2018 - 2019*
- Scraped and processed data from various scientific databases to populate knowledge graphs. Engineered ontologies for the extracted data.

Awards and grants

Scholarships:

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

McGill Departmental Award (6 000$) *2021 - 2025*

DeepMind Masters Scholarship (12 000$) *2020 - 2021*

Grants:

Samsung SAIT Call for Projects, PIs : Siamak Ravanbakhsh and Yoshua Bengio (60 000$) *2022*

Awards:

Laureate of the Acfas science popularization contest *2018*

Research

Publications

Conference papers:

A. K. Mondal, S. Panigrahi, **S.-O. Kaba**, S. Rajeswar, S. Ravanbakhsh.
Equivariant adaptation of large pre-trained models, NeurIPS 2023.

S.-O. Kaba*, A. K. Mondal*, Y. Zhang, Y. Bengio, S. Ravanbakhsh.
Equivariance with learned canonicalization functions, ICML 2023.

S.-O. Kaba, S. Ravabakhsh.
Equivariant networks for crystal structures, NeurIPS 2022.

M. Pezeshki, **S.-O. Kaba**, Y. Bengio, A. Courville, D. Precup, and G. Lajoie.
Gradient starvation: A learning proclivity in neural networks, NeurIPS 2021.

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, Physical Review Materials 2023.

S.-O. Kaba and D. Sénéchal.
Group-theoretical classification of superconducting states of strontium ruthenate, Physical Review B 2019.

Peer-reviewed workshop papers:

D. Levy*, S. Panigrahi*, **S.-O. Kaba***, Q. Zhu, K. Lee, M. Galkin, S. Miret, S. Ravanbakhsh.
SymmCD: Symmetry-preserving crystal generation with diffusion models, NeurIPS 2024 AI4Mat workshop. **(Oral)**

H. Lawrence, V. Portilheiro, Y. Zhang, **S.-O. Kaba**.
Improving equivariant networks with probabilistic symmetry breaking, ICML 2024 GRaM workshop.

S.-O. Kaba, S. Ravanbakhsh.
Symmetry breaking and equivariant neural networks, NeurIPS 2023 NeurReps workshop. (**Oral**)

S.-O. Kaba*, A. K. Mondal*, Y. Zhang, Y. Bengio, S. Ravanbakhsh.
Equivariance with learned canonicalization functions, NeurIPS 2022 NeurReps workshop. **(Oral)**

D. Levy*, **S.-O. Kaba***, C. Gonzales, S. Miret, S. Ravanbakhsh.
Using multiple vector channels improves E(n)-equivariant graph neural networks, ICML 2023 Workshop on ML for Astrophysics.

Work under review:

D. Levy*, S. Panigrahi*, **S.-O. Kaba***, Q. Zhu, K. Lee, M. Galkin, S. Miret, S. Ravanbakhsh.
SymmCD: Symmetry-preserving crystal generation with diffusion models, Under review at ICLR 2025.

H. Lawrence, V. Portilheiro, Y. Zhang, **S.-O. Kaba**.
Improving equivariant networks with probabilistic symmetry breaking, Under review at ICLR 2025.

X. Li, **S.-O. Kaba**, S. Ravanbakhsh.
On the identifiability of causal abstractions, Under review at AISTATS 2025.

Selected presentations

Advances in deep learning for materials discovery. IBM Quantum, 2024.

AI for materials discovery. Deep Learning IndabaX, 2024. (**Keynote**)

Valoriser les communautés noires en IA. IVADO, 2022. (**Panel**)

Equivariant networks for crystal structures. Learning on Graphs Conference, 2022.

Superconductivity in Sr_2RuO_4 with quantum cluster methods. CGQC, 2018. (**Best presentation award**)

Technical skills

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

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

Supervision and teaching

Internship co-supervisor
Supervised the internship of Jikael Gagnon during my PhD *2024*

Internship co-supervisor
Supervised the internship of Jonathan Clepkens during my masters *2018*

Teaching Assistant
Université de Sherbrooke *2017*
Course: Statistical Mechanics I

Professional service

Reviewing and Workshop organization

Workshop Organizer and Program Chair
ICML 2024 workhop on Geometry-grounded Representation Learning and Generative Modeling *2024*

Reading Group Organizer
Geometric Deep Learning Reading Group *2023 - 2024*

Reviewer
Reviewed for NeurIPS, ICML, ICLR, AAAI, Science Advances, Nature Machine Intelligence

Outreach

Science Communication Consultant
Acfas *Since 2019*

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

Science Popularizer
Boîte à science *2014*

Leadership positions

Laboratory Representative
Mila - Quebec Artificial Intelligence Institute *2020 - 2022*

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

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