Sékou-Oumar Kaba

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Machine learning Ph.D. student with a physics background and software engineering experience. My research 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 for prediction and generation tasks.

Master of Science in Physics — **Sherbrooke**
Université de 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 — *2023*
Supervisor: Dr. Giulia Luise

Research Intern in Machine Learning — **Montréal**
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 development of data collection, analysis, and visualization software, with applications in geolocation, NLP and computer vision.

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:

(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*, 2024.

(Under review) H. Lawrence, V. Portilheiro, Y. Zhang, **S.-O. Kaba**. *Improving equivariant networks with probabilistic symmetry breaking*, 2024.

(Under review) X. Li, **S.-O. Kaba**, S. Ravanbakhsh. *On the identifiability of causal abstractions*, 2024.

A. K. Mondal, 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.

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, 7:044407, 2023.

S.-O. Kaba and D. Sénéchal. *Group-theoretical classification of superconducting states of strontium ruthenate.* Physical Review B, 100:214507, 2019.

Workshop papers:

H. Lawrence, V. Portilheiro, Y. Zhang, **S.-O. Kaba**. *Improving Equivariant Networks with Probabilistic Symmetry Breaking.* ICML Workshop on Geometry-grounded Representation Learning and Generative Modeling, 2024.

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. (**Oral**)

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.

Presentations, invited talks and panels:

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

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

AI for materials discovery. Quantum and AI Day, Canada, 2024.

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

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

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

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:

Best presentation award, CGQC *2018*

Laureate of the Acfas science popularization contest *2018*

Grants

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

Technical skills

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

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

Other experience

Academic

ICML 2024 Workshop on Geometry-grounded Representations and Generative Modeling

Co-organized the GRaM workshop at ICML *2024*

Geometric Deep Learning Reading Group

Co-organized the Geometric Deep Learning Reading Group at Mila *2023-2024*

Quantum and AI Day at Mila

Co-organized the Quantum and AI Day at Mila *2023*

Reviewer

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

Teaching

Teaching Assistant **Sherbrooke**

Université de Sherbrooke *2017*

Course: Statistical Mechanics I

Science Instructor **Québec**

Cégep de Sainte-Foy *2013 - 2015*

Outreach

Science Communication Consultant **Montréal**

Acfas *Since 2019*

Radio Host **Montréal**

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 **Québec**

Boîte à science *2014*

Community service

Laboratory Representative **Montréal**

Mila - Quebec Artificial Intelligence Institute *2020 - 2022*

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*