

Dr. Astrid P. Klipfel

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Personal information

Birth	📅	June 19, 1997
Nationality	📅	French
DBLP	📅	https://dblp.org/pid/326/8986.html
Scholar	📅	https://scholar.google.com/citations?hl=en&user=-gNXRYQAAAAJ

Current position

Temporary teaching and research assistant (ATER) at Université d'Artois, France

Previous positions

2020	📅	Internship , Deep learning for MIR, MINELab (NCU), Taiwan
2018-2019	📅	Internship , Electronics design, data collection and analysis, Innovation Crunch Lab, France

Education

2020 – 2023	📅	Ph.D. in computer science, Université d'Artois Thesis title: <i>Design of new semiconducting electrodes for photoelectrochemical energy conversion by machine learning and DFT calculations</i>
2015 – 2020	📅	Computer science engineer, UTBM (Université de technologie de Belfort Montbéliard)

Grants

2023-2027	📅	ANR JCJC ERIANA , Event-Centric Reasoning for Interpreting Everyday Narratives, member
2021-2022	📅	CNRS FEI EMILIE , Explainable Multi-label few-shot Image Classification with qualitative constraint networks and word Embeddings, member
2020-2025	📅	ANR VIVAH , Vers une Intelligence Artificielle à Visage Humain, member


Supervision of graduate students

2023-2026	📅	Supervision of Elohan Veillon on his thesis entitled: <i>Design of diffusion-based generative models for the discovery of new crystallographic structures</i> at Artois University
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Teaching activities

2020-2024	📅	Algorithm Undergraduate program, Computer Science department, tutorials and labs session
2023	📅	C language Undergraduate program, Computer Science department, labs session
2022, 2024	📅	Object-Oriented Programming Undergraduate program, Computer Science department, tutorials and labs session
2023-2024	📅	Machine learning applied to Biochemistry Graduate program, Biologie department, lectures and labs session


Teaching activities (continued)

2024  **Machine learning** Graduate program, Computer Science department, lectures and labs session

Service to the scientific community

AAAI 2024  PC membre
UAI 2023  PC membre
ECAI 2024  PC membre
IJAR  Reviewer, International Journal of Approximate Reasoning

Organisation of scientific meetings

ESQARU 2023  Staff member, *17th European Conference on Symbolic and Quantitative Approaches to Reasoning with Uncertainty*

Talks

Invited talks

1 A. Klipfel, Z. Bouraoui, Y. Fregier, and A. Sayede, *Equivariant graph neural network for crystalline materials*, 2022.

Chemistry conferences



1 A. Klipfel, Z. Bouraoui, O. Peltre, Y. Fregier, and A. Sayede, "Periodic equivariant graph neural network (pegnn) for crystalin system," 2022.

Publications

Conference Proceedings

- 1 A. Klipfel, Y. Fregier, A. Sayede, and Z. Bouraoui, "Vector field oriented diffusion model for crystal material generation," in *Proceedings of the AAAI Conference on Artificial Intelligence*, 2024.
- 2 A. Klipfel, Z. Bouraoui, Y. Fregier, and A. Sayede, "Optimized crystallographic graph generation for material science," in *32st International Joint Conference on Artificial Intelligence*, 2023.
- 3 A. Klipfel, Z. Bouraoui, Y. Fregier, and A. Sayede, "Unified model for crystalline material generation," in *32st International Joint Conference on Artificial Intelligence*, 2023.
- 4 A. Klipfel, Z. Bouraoui, O. Peltre, Y. Fregier, N. Harrati, and A. Sayede, "Equivariant message passing neural network for crystal material discovery," 12, vol. 37, Jun. 2023, pp. 14 304–14 311.

Tools

python package  **Crystallographic graph**, Graph construction on GPU for Materials Science, <https://github.com/aklipf/mat-graph>
 **Materials toolkit**, A python package for machine learning in Materials Science, <https://github.com/materials-toolkits/pymaterials>