Lisa **BEREZOVSKA**

RESEARCH SCIENTIST IN MOLECULAR DYNAMICS

Computational scientist with a PhD in Physics and postdoctoral experience in Structural Biology. Skilled in MD simulations, Python-based data analysis. Interested in applying advanced MD simulations, enhanced sampling, and AI-assisted modelling to drug discovery and molecular design.

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Montpellier

www.linkedin.com/in/llisabere

Open to remote work

Computer skills

Languages and libraries
Python (NumPy, pandas, seaborn), bash, SQL

Tools
Slurm, OpenMM, GROMACS, LAMMPS, PLUMED, VMD, Ovito

Machine Learning (in progress)
scikit-learn, PyTorch

Languages

English
C1 (TOEIC 975/990)

French
B1

Ukrainian

Assets

Curiosity

Adaptability & Fast learning

Capacity to resolve complex problems

Analytical mindset

Interests

Yoga, Boxing

Reading, Photo

Work experience

Postdoc in Structural Biology Jan. 2023 - Jun. 2025 **(2 years+)**
INSERM, Centre de Biologie Structurale, Montpellier, France

- Designed, executed, and analysed **molecular dynamics simulations** of short peptides and protein condensates at all-atom and coarse-grained levels
- Developed **Python-based analysis pipelines** for trajectory processing, metric extraction, and structural visualisation
- Explored different force fields (AMBER and CHARMM families) in regards to protein aggregation
- Applied **metadynamics** and **replica exchange** to enhance sampling of condensate states
- Optimised **HPC simulation workflows** (SLURM) to reduce computational time by 5% and improve reproducibility
- Implemented an analysis tool in **OpenMM** for predicting beta structures (ELF3)
- Explored RNA-protein interactions through the dynamics of condensates enriched in charged residues
- Collaborated with 4 international research groups and contributed to 2 peer-reviewed publications

Environment: Python, MDAnalysis, NumPy, OpenMM, GROMACS, Bash, Slurm

Main Skills

Statistical analysis

Data analysis (Python, Excel)

Visualisation and reporting (seaborn)

Scientific communication

Education

PhD in Physics 2019 - 2022
Université de Strasbourg, Institut Charles Sadron (France),
Thesis: Non-ideal mixing of phospholipid membranes: Molecular Dynamics perspective

Master in physics of condensed matter and nano physics 2018 - 2019
Université de Strasbourg (France),

Erasmus Exchange 2017 - 2018
Université d'Aston (Royaume-Uni),

Bs in Physics 2013 - 2017
Université nationale Taras Schevchenko de Kiev (Ukraine),

Certifications

SQL (Mimo 2025)

Artificial Intelligence Fundamentals (IBM SKillsBuild 2025)

Google AI Essential V1 (Google 2025)

Personal Projects

- Exploratory analysis of russian strikes with pandas & seaborn
- Classification of images of cats/dogs with PyTorch
- Preprocessing pipeline and supervised classification (IBM project)