Lisa **Berezovska**

Modeling · Molecular Dynamics · Protein Interactions & Aggregation

Montpellier, France

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Python	pandas, scipy, seaborn, MDAnalysis, mdtraj
Simulation	GROMACS, LAMMPS, OpenMM, PLUMED
Modeling	AlphaFold Server, AlphaFold Multimer
Visualization	VMD, ChimeraX, Ovito
Other	Unix/bash, slurm, Git

Experience

Inserm, Centre de Biologie Structurale — *Montpellier, France*

Postdoctoral Researcher — *Jan 2023 - Jun 2025*

Phase Separation of Short Peptides

- Studied aggregation of short motif of FUS protein that is to neurodegenerative diseases as ALS
- Made the first all-atom resolution phase coexistance simulation with sampling of both dilute and dense phases in sub micro second timescales
- Implemented a graph-based clustering algorithm to recognize dense, interfacial and dilute phases of peptides
- Determined that replica-exchange and metadynamics enhanced sampling methods do not improve sampling efficiency of multi component short peptides systems
- Collaborated with wet lab and AFM researchers to compare reliability of modern force fields - amber family showed good agreement with experiment (errors: 20% on density and 5% on dilute phase diffusion)
- Increased simulation speed by 5% on ADASTRA HPC via slurm parameter optimization
- Developed Python tools to assess convergence, diffusion coefficients, and interaction patterns across multi-phase systems

Early Flowering Plant Protein

- Performed coarse-grained simulations using CALVADOS force field for ELF3 protein
- Implemented in OpenMM a secondary structure algorithm to mimic formation of beta sheets

RNA condensates

- Studied arginine and lysine rich RNA condensates and found comparable contact lifetimes in both cases

Education

University of Strasbourg, Institut Charles Sadron — *Strasbourg, France*

PhD in Physics — *Oct 2019 - Dec 2022*

Thesis: Non-ideality of mixing in phospholipid bilayer system: molecular dynamics view

Studied model mixtures of phospholipids in a bilayer with cholesterol and quantified their Flory-Huggins interaction parameters using theory of regular solutions. Performed MD simulations in LAMMPS with SPICA CG force field, developed Python analysis scripts and theoretical framework to study complex mixtures using Kirkwood-Buff approach. Self-mixing of phospholipids was 50% higher compared to mixing with cholesterol.

University of Strasbourg, Institut de Physique et Chimie des Matériaux — *Strasbourg, France*
Taras Schevchenko National University of Kyiv — *Kyiv, Ukraine*

MS in Condensed Matter and Nanophysics / MS in Molecular Physics — *Sep 2018 - Jul 2019*

Thesis: Computational Study of Crystallization of Chain Molecules

Studied phase behavior of polymer systems using Monte Carlo simulations and found that shorter chain lengths increased crystallization efficiency in the CG-PVA coarse-grained model by 15%.

Aston University *Birmingham, UK*
Taras Schevchenko National University of Kyiv *Kyiv, Ukraine*
Erasmus Exchange *Sep 2017 - Jul 2018*
Course Project: Implementation of Hybrid Hydro Molecular Dynamics into classical MD in GROMACS

Taras Schevchenko National University of Kyiv *Kyiv, Ukraine*
BS in Physics *Sep 2013 - Jul 2017*
Thesis: Influence of the intermolecular interaction potential anisotropy on the equilibrium of model liquids
Studied vapor-liquid equilibrium and surface tension using Wang-Landau method with in-house MD simulation. Found that the influence of anisotropy does not exceed statistical noise.

Scientific Outreach

Strasbourg Soft Matter Days *Strasbourg, France*
Organizing Committee *Jun 2021 / Jun 2022*
Co-organized a two-day conference on soft matter physics for 25 presenters and $\sim$ 100 attendees. Scheduled talks, procured badges and moderated events' web page.

Publications

Influence of the intermolecular interaction potential anisotropy on the surface tension of model liquids *Ukr. J. Phys.* *Jun 2025*
Berezovska Y.O., Grygoryev A.N., Gavryushenko D.A.

Exploring RNA Destabilization Mechanisms in Biomolecular Condensates through Atomistic Simulations *PNAS* *Apr 2025*
Boccalini M., Berezovska Y., Bussi G., Paloni M., Barducci A.

Non-ideal mixing of lipids: a molecular dynamics perspective *J. Chem. Phys.* *Feb 2025*
Berezovska L., Kociurzynski R., Thalmann F.

Internal lipid bilayer friction coefficient from equilibrium canonical simulations *J. Phys. Commun.* *Jan 2022*
Benazieb O., Berezovska L., Thalmann F.

Conferences

Talks

FEBS Protein Dynamics Workshop 2024 *Les Houches, France*
YRS Seminars 2023 / 2024 *Montpellier, France*
LLPS Seminars 2023 *Montpellier, France*
DPG Spring Meeting of the Condensed Matter Section 2022 *Regensburg, Germany*
Strasbourg Soft Matter Days 2021 / 2022 *Strasbourg, France*
Ecole Doctorale PhD conference 2021 / 2022 *Strasbourg, France*
APS Match Meeting 2022 *(online) Chicago, USA*

Posters

CECAM Workshop: Bridging the Atomic-Mesoscale Gap for Complex Interfaces 2024 *Montpellier, France*
International Soft Matter Summer School 2022 *Cargese, France*