

Eleftherios Mainas

POSTDOCTORAL RESEARCHER AT THE PIERILAB · UNC@CHAPELHILL

Chapel Hill, North Carolina

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Education

Brown University

Providence, RI

PHD CHEMISTRY

2018 - 2023

- Advisor: Dr. Richard M. Stratt
- Thesis: Large-Deviation Theory Approach to Systems with Orientational Order: Results for Two and Three Dimensional Liquid Crystals

University of Athens

Athens, Greece

BS CHEMISTRY

2013 - 2017

- Advisor: Dr. Zoe Cournia
- Thesis: Modeling magnetic nanoparticles coated with polyvinyl alcohol and polyarabic acid in contact with model cell membranes.

Research Experience

University of North Carolina at Chapel Hill - Department of Chemistry

Chapel Hill, NC

ADVISOR: DR. ELISA PIERI

2023-now

- I developed a **statistical mechanical microstate model** for the titration states of the chromophore biliverdin inside the protein Sandercyanin. **Constant pH Molecular Dynamics** in combination with **QM/MM** were able to reveal the key role of biliverdin in the protein's oligomerization state. Preventing the protein from forming oligomers will unlock its full potential for bioimaging.

Brown University - Department of Chemistry

Providence, RI

ADVISOR: DR. RICHARD STRATT

2019-2023

- Using **large-deviation theory**, I described an approach to computing expressions for orientational order probability distributions that make use of simulation information to accurately compute even the large fluctuation limit of these distributions. The key is to think about the limiting extremes of the system's response to an applied field. When the field is weak, the central-limit theorem applies, but in the presence of a strong field, individual rotors feel a mean-field from the rest of the system. Simple **Pade' interpolation** between these limits and a subsequent **thermodynamic integration** generated accurate orientational probability distributions from simulation.

BRFAA - Biomedical Research Foundation Academy Of Athens

Athens, Greece

SUPERVISOR: DR. ZOE COURNIA

2016-2018

- **All-atom molecular dynamics simulations** were performed to study polymer-coated **magnetic nanoparticles** (MAG-PVA and MAG-ARA) near a **DPPC lipid bilayer**. Both nanoparticles showed bimodal diffusion, remained outside the bilayer, and caused lipid head group ordering and reduced area per lipid. MAG-PVA interacted more strongly and stayed closer to the bilayer than MAG-ARA.

Teaching Experience

Fall & Spring 2023	Equilibrium, Rate, and Structure Lab , Lab Supervisor	Brown University
Spring 2020-2022	Statistical Mechanics , Teaching Assistant	Brown University
Fall 2019-2022	Quantum Mechanics , Teaching Assistant	Brown University

Publications

PUBLISHED

Mainas E., et al. Exceptionally Large Fluctuations in Orientational Order: The Lessons of Large-Deviation Theory for Liquid Crystalline Systems. *J. Chem. Phys.* 162, 024501 (2025). [\[First author\]](#)

Mainas E., et al. Biliverdin's Propionic Chains Influence Oligomerization in Sandercyanin. *J. Phys. Chem. B* 128, 50, 12443-12455 (2024). [\[First author\]](#)

Mainas E., et al. Coating of magnetic nanoparticles affects their interactions with model cell membranes. *Biochimica et Biophysica Acta (BBA)-General Subjects* 1864 (11), 129671 (2020). [\[First author\]](#)

IN PREP

Mainas E., et al. Large-deviation theory perspective on two and three-dimensional polymer end-to-end distances. *J. Chem. Phys.* [\[First author\]](#)

Mainas E., et al. Protonation dependent binding of Biliverdin to various protein environments. *J. Phys. Chem. B* [\[First author\]](#)

Awards, Fellowships, & Grants

2024	Postdoctoral Excellence Award , UNC at Chapel Hill	<i>No monetary prize</i>
2024	Best Poster Award , American Conference on Theoretical Chemistry	\$ 200
2024	Travel Grant , Amber Developer Meeting in Tampa, Florida	\$ 1,500
2022	Graduate Research Fellowship , American Hellenic Educational Progressive Association	\$ 5,000
2021	Potter Prize - Travel Grant , Brown University	\$ 2,000
2018-2023	Graduate School Fellowship , Brown University	\$ 450,000
2017	Best Poster Award , Hellenic Society for Computational Biology	<i>No monetary prize</i>
2016	Computational Grant , Greek Research & Technology Network	650,000 core-hours

Posters and Presentations

Mainas E., et al. 2024. Constant pH Molecular Dynamics of the Sandercyanin-Biliverdin Complex. *Poster*, American Conference on Theoretical Chemistry.

Mainas E. 2023. Large-Deviation Theory Approach to Systems With Orientational Order: Results for Two and Three Dimensional Liquid Crystals. *Presentation*, Biomedical Research Foundation Academy Of Athens.

Mainas E. 2022. A novel diagnostic tool for RNA force field inefficiencies: The case of gcUUCGgc folding. *Original Research Proposal*, Brown University.

Mainas E., et al. 2022. Novel Theory of the Orientational Order of Finite Disordered Systems: Results for 2D Liquid Crystals. *Poster&Presentation*, Berkeley Statistical Mechanics Meeting.

Mainas E., et al. 2017. Coating of magnetic nanoparticles affects their interactions with model cell membranes. *Poster&Presentation*, Hellenic Society for Computational Biology.

Mentoring

- 2024-Now **Kendall Cherry**, Graduate Student, University of North Carolina at Chapel Hill
- 2023-Now **Noureen Abdelrahman**, Graduate Student, University of North Carolina at Chapel Hill
- 2023-Now **Kaiyi Tong**, Graduate Student, University of North Carolina at Chapel Hill
- 2023-Now **Shaena Riddles**, Undergraduate Student, University of North Carolina at Chapel Hill
- 2018-2019 **Andrew Ton**, Undergraduate Student, Brown University
- 2016-2017 **Nephele Agrafiotis**, Undergraduate Student, University of California, Los Angeles

Outreach & Professional Development

SERVICE AND OUTREACH

- 2023 **Rhode Island Science and Engineering Fair**, Volunteer Judge
- 2025 **North Carolina Science and Engineering Fair**, Volunteer Judge

DEVELOPMENT

Workshop, Gaussian accelerated Molecular Dynamics (GaMD), University of North Carolina (UNC), Chapel Hill. 2024.

Certification, ACS Reviewer Lab. 2024.

Software, Amber development team. 2024.

Blogging, emainas.github.io

PEER REVIEW

Journal of Chemical Information and Modeling

References

- 2023-Now **Elisa Pieri**, elipieri@unc.edu
- 2018-2023 **Richard Stratt**, richard_stratt@brown.edu
- 2018-2023 **Brenda Rubenstein**, brenda_rubenstein@brown.edu