Roja **Rahmani**

PH.D. CANDIDATE IN PHYSICAL CHEMISTRY

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Summary

I am a physical and computational chemist with years of experience in enhanced sampling in MD simulations and studying the bio-nano interface and surface properties. I have independently initiated an interdisciplinary project and led an international collaboration combining computational and experimental work. I have been actively involved in teaching two courses throughout my Ph.D., as well as supervising a bachelor's student for her thesis and bachelor project. I am also a former member of the Ph.D. council.

Education

Stockholm University — *Stockholm, Sweden*

PH.D. IN PHYSICAL CHEMISTRY (DEFENDING SOON) — *Oct 2020 – Present*

- **Supervisor: Prof. Alexander Lyubartsev**
- Focused on bio-nano interface properties and **biomolecular adsorption to nanomaterials** using various enhanced sampling **MD simulations** methods including the Metadynamics method.

K. N. Toosi University of Technology — *Tehran, Iran*

M.SC. IN PHYSICAL CHEMISTRY — *2016 – 2019*

- Thesis title: *Study of the interaction of ZnS nanosheets and nanotubes with amino acids using computer modeling.*

University of Tabriz — *Tabriz, Iran*

B.SC. IN APPLIED CHEMISTRY — *2013 – 2016*

Publications

[1] Rahmani, R., Lyubartsev, A. P. (2025). Uncovering sequence effects in Titanium binding peptides adsorption on TiO_2: A molecular dynamics study. *Scientific Reports*, 15(1), 26885.

[2] Saeedimasine, M., Rahmani, R., Lyubartsev, A. P. (2024). Biomolecular adsorption on nanomaterials: combining molecular simulations with machine learning. *Journal of Chemical Information and Modeling*, 64(9), 3799-3811.

[3] Rahmani, R., Lyubartsev, A. P. (2023). Biomolecular adsorprion at ZnS nanomaterials: A molecular dynamics simulation study of the adsorption preferences, effects of the surface curvature and coating. *Nanomaterials*, 13(15), 2239.

Experience

Stockholm University — *Sweden*

PH.D. STUDENT — *Oct 2020 – Present*

- Conduct computational studies on bio–nano interface interactions and biomolecular adsorption to different surfaces using MD simulations and several enhanced sampling methods.
- Programming (Python) for data analysis.
- Designed and led a project to uncover sequence-dependent binding mechanisms of titanium-binding peptides.
- Developed collaborations with experimental and computational groups.
- Wrote proposals for funding my research exchange and international conference participations.

Sweden

Teaching Assistant *2021 – 2025*

- For Physical Chemistry (Quantum Mechanics, Spectroscopy) and Chemical Bonding courses.
- Responsibilities: conducted calculation exercise sessions, lectures for each lab's theoretical concepts, improving lab compendiums, led tutorials, helping students to conduct computational and experimental labs, provided feeback for students' lab reports, and for undergraduate courses, observed exams for undergraduate courses.

Sweden

Ph.D. Council *2021*

- Organized events for fellow Ph.D. students, supported their concerns, and served as a liaison between the student body and the department leadership as a member of the Departmental Board.

Nottingham Trent University *United Kingdom*

Visiting Ph.D. Student *Mar 2025 – May 2025*

- Conducted experimental work on peptide adsorption to titanium surfaces using QCM-D.
- Synthesized peptides via solid-phase peptide synthesis (SPPS).
- Investigated adsorption under varying pH and 0.15 M NaCl to model physiological conditions.
- Integrated computational predictions with experimental validation of peptide–surface interactions.

Supervision and Mentoring

- Supervised a Bachelor's student on a project and thesis focused on ***pH-dependent adsorption of amino acids on TiO_2 surfaces using molecular simulations*** (Spring 2024). Also provided scientific help for new lab members and visiting students in the group.

Presentations

2025, 11-13 June **Oral presentation**, eSSENCE-EMMC Multiscale meeting *Uppsala, Sweden*

2024 **Oral presentation**, CECAM Workshop on Peptides in Biology and Materials *Florence, Italy*

2024 **Poster presentation**, 37th European and 14th International Peptide Symposium *Florence, Italy*

2023 **Oral presentation**, NANOSOLVEIT Conference *Piraeus, Greece*

2023 **Poster presentation**, CECAM-GGMM Young Modeller Conference *Toulouse, France*

2022 **Poster presentation**, eSSENCE-EMMC Multiscale meeting *Uppsala, Sweden*

Awards and Scholarships

2024 **Visiting Researcher Scholarship**, Stockholm University Center for Circular and Sustainable Systems (SUCCeSS) *Sweden / Nottingham Trent University, UK*

2024 **Chemistry Scholarship**, Royal Swedish Academy of Sciences *Sweden*

2024 **Liljevalch J:or's Travel Grant**, Stockholm University *Sweden*

2023 **Hilda Rietz Scholarship**, Royal Swedish Academy of Sciences *Sweden*

2023 **Donation Scholarship**, Stockholm University *Sweden*

References

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Stockholm University

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