

Ayşenur İşcen Akatay

Department of Chemistry – Boğaziçi University, 34342 Bebek/İstanbul, Türkiye

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Profile

- o Chemical engineer highly experienced in computational chemistry, molecular modeling and simulation methods, including *ab initio* quantum chemistry methods, atomistic and coarse-grained molecular dynamics simulations.
- o Research interests include multi-scale modeling of bioinspired materials, self-assembly, supramolecular chemistry and polymer physics

Education

Northwestern University

September 2014 – September 2019

Ph.D., Chemical and Biological Engineering

Advisor: Prof. George C. Schatz

Thesis: Design of Stimuli-Responsive Bioinspired Materials using Computational Methods

Yeditepe University

September 2011 – June 2014

Bachelor of Science, Chemical Engineering

GPA: 3.91/4.0 Class rank: 1st in Faculty of Engineering and Architecture

Professional Experience

Assistant Professor

December 2024 – Present

Boğaziçi University

Chemistry Department

TÜBİTAK 2232 Fellow

August 2023 – November 2024

Sabancı University

Investigation of structure-property relationships in amyloid-like supramolecular peptide nanofibrils

Postdoctoral Researcher

September 2019 – June 2023

Max Planck Institute for Polymer Research

Advisor: Prof. Dr. Kurt Kremer

- o One of the work package leaders in Active & intelligent PACKaging materials and display cases as a tool for preventive conservation of Cultural Heritage (APACHE) project funded by EU Horizon 2020
- o Designed multi-scale simulation strategies to study degradation processes of acrylic paints in modern artwork
- o Presented work in workshops and public training sessions

Research Assistant

September 2014 – September 2019

Northwestern University Chemical and Biological Engineering Department

- o Developed molecular modeling methods for studying self-assembly and dynamic properties of bioinspired materials

- o Conducted research projects in collaborative research centers:
 - Center for Bio-Inspired Energy Sciences (CBES)
 - Advanced Materials for Energy-Water Systems Centers (AMEWS)
 - Center for Computation and Theory of Soft Materials (CCTSM)

Teaching Assistant

September 2014 – September 2019

Northwestern University Chemical and Biological Engineering Department

- o Held lectures in absence of instructor
- o Held weekly office hours and review sessions
- o Graded homework assignments and projects
- o Courses TA'd:
 - Heat Transfer – Winter 2018
 - Phase Equilibrium and Staged Separations – Spring 2017
 - Mass Transfer – Spring 2015, 2016

Research Intern

June – July 2013

TÜBİTAK (The Scientific and Technological Research Council of Turkey), Marmara Research Center, Gebze/Kocaeli

- o “Development of Warm-mix Asphalt Additives Production Technology”- Analyzed synthesized materials, performed softening point tests of asphalt samples
- o “Production of Palladium Catalysts for Hydrogen Oxidation”-Synthesized and tested palladium catalysts
- o Chemistry Institute Industrial Services Department - Performed chemical analyses for industrial mineral oil samples

Engineering Intern

August 2013

EVYAP A.S., Tuzla, Istanbul

- o Research and Development Department- Developed formulations and optimizations processes for personal care products

Achievements

TÜBİTAK 2232-B International Fellowship for Early Stage Researchers	2023
Northwestern University Hierarchical Materials Cluster Program Fellowship	2016
Yeditepe University High Honors	2014
Yeditepe University Full Scholarship	2011 – 2014

Publications

Published or Accepted Manuscripts

15. **A. Iscen**, K. Kaygisiz, C. V. Synatschke, T. Weil, K. Kremer, Multiscale Simulations of Self-Assembling Peptides: Surface and Core Hydrophobicity Determine Fibril Stability and Amyloid Aggregation, *Biomacromolecules*, 25 (5), 3065-3075 (2024), DOI: 10.1021/acs.biomac.4c00151
14. K. Kaygisiz, L. Rauch-Wirth, **A. Iscen**, J. Hartenfels, K. Kremer, J. Münch, C. V. Synatschke, T. Weil, Peptide amphiphiles as biodegradable adjuvants for efficient retroviral gene delivery, *Advanced Healthcare Materials*, 2301364 (2023), DOI: 10.1002/adhm.202301364
13. A. Banerjee, **A. Iscen**, Kurt Kremer, Oleksandra Kukharenko, Determining glass transition in all-atom acrylic polymeric melts simulations using machine learning, *J. Chem. Phys.*, 159, 074108 (2023), DOI: 10.1063/5.0151156
12. C. Li, Q. Xiong, T. D. Clemons, H. Sai, Y. Yang, M. H. Sangji, **A. Iscen**, L. C. Palmer, George C. Schatz, S. I. Stupp, Role of Supramolecular Polymers in Photo-actuation of Spiropyran Hydrogels, *Chemical Science* 14, 6095-6104 (2023), DOI: 10.1039/D3SC00401E
11. **A. Iscen**, N. C. Forero-Martinez, O. Valsson, and K. Kremer, Molecular Simulation Strategies for Understanding the Degradation Mechanisms of Acrylic Polymers, *Macromolecules* 56 (9), 3272-3285 (2023), DOI: 10.1021/acs.macromol.2c02442
10. **A. Iscen**, N. C. Forero-Martinez, O. Valsson, and K. Kremer, Acrylic Paints: An Atomistic View of Polymer Structure and Effects of Environmental Pollutants, *J. Phys. Chem. B* 125 (38), 10854-10865 (2021), DOI: 10.1021/acs.jpcc.1c05188
9. E. Barry, R. Burns, ..., **A. Iscen**, ..., S. B. Darling, Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport, *Chemical Reviews* 121 (15), 9450-9501 (2021), DOI: 10.1021/acs.chemrev.1c00069
8. C. Li, **A. Iscen**, H. Sai, K. Sato, N. A. Sather, S. M. Chin, Z. Alvarez, L. C. Palmer, G. C. Schatz and S. I. Stupp, Supramolecular-covalent hybrid polymers for light-activated mechanical actuation, *Nat. Mater.* 19, 900-909 (2020). <https://doi.org/10.1038/s41563-020-0707-7>
7. N. H. C. Lewis, **A. Iscen**, A. Felts, B. Dereka, G. C. Schatz, and A. Tokmakoff, Vibrational Probe of Aqueous Electrolytes: The Field Is Not Enough, *J. Phys. Chem. B* 124 (32), 7013-7026 (2020), DOI: 10.1021/acs.jpcc.0c05510
6. C. Li, **A. Iscen**, L. C. Palmer, G. C. Schatz, and S. I. Stupp, Light-Driven Expansion of Spiropyran Hydrogels, *J. Am. Chem. Soc.* 142 (18), 8447-8453 (2020). DOI: 10.1021/jacs.0c02201
5. D. Samanta, **A. Iscen**, C. R. Laramy, S. B. Ebrahimi, K. E. Bujold, G. C. Schatz, C. A. Mirkin, Multivalent Cation Induced Reversible Actuation of Colloidal Superlattices, *J. Am. Chem. Soc.* 141 (51), 19973-19977 (2019). DOI: 10.1021/jacs.9b09900
4. **A. Iscen**, C. R. Brue, K. F. Roberts, J. Kim, G. C. Schatz, T. J. Meade, Inhibition of Amyloid- β Aggregation by Cobalt(III) Schiff Base Complexes: A Computational and Experimental Approach, *J. Am. Chem. Soc.* 141 (42), 16685-16695 (2019). DOI: 10.1021/jacs.9b06388

3. **A. Iscen**, G. C. Schatz, Hofmeister Effects on Peptide Amphiphile Nanofiber Self-Assembly, *J. Phys. Chem. B* 123 (32), 7006-7013 (2019). DOI: 10.1021/acs.jpcc.9b05532
2. B. J. Hong, **A. Iscen**, A. J. Chipre, M. M. Li, One-Sun Lee, J. N. Leonard, G. C. Schatz, S. B. T. Nguyen, Highly stable, ultrasmall polymer-grafted nanobins (usPGNSs) with stimuli-responsive capability, *J. Phys. Chem. Lett.* 9, 1133-1139 (2018). DOI: 10.1021/acs.jpclett.7b03312
1. **A. Iscen**, G. C. Schatz, Peptide amphiphile self-assembly, *EPL* 119, 38002 (2017). DOI:10.1209/0295-5075/119/38002

Conference Presentations

3. **Aysenur Iscen**, N. C. Forero-Martinez, O. Valsson, and K. Kremer, "Acrylic Paints: An Atomistic View of Polymer Structure and Effects of Environmental Pollutants", Focus Session Speaker at American Physical Society National Meeting, March 2022.
2. **Aysenur Iscen**, George C. Schatz, "Supramolecular Peptide Amphiphile Polymeric Hybrid Hydrogels for Photo- actuation: Modeling and Simulation", Poster presentation delivered at American Chemical Society National Meeting, March 2019.
1. **Aysenur Iscen**, Chuang Li, Liam Palmer, Samuel I. Stupp, George C. Schatz, "Supramolecular Peptide Amphiphile Polymeric Hybrid Hydrogels for Photo- actuation: Modeling and Simulation", Poster presentation delivered at Bio-inspired Materials Gordon Research Conference, Les Diablerets, Switzerland, June 2018.

Computer Skills

Computational Chemistry Software

NAMD, GROMACS, Amber, PLUMED, LAMMPS, Gaussian, GAMESS, VMD

Others

Python, Tcl/Tk, MATLAB, L^AT_EX, Microsoft Office

Professional Memberships and Service

American Chemical Society	2019-
Member	
American Physical Society	2021-
Member	
Reviewer in academic scientific journals	2019-
o Polymer	
o Journal of Physical Chemistry B	
o Journal of Physical Chemistry C	
o Journal of Industrial & Engineering Chemistry	

Community Outreach

Department of Energy Basic Energy Sciences	2018-2019
Early Career Network Representative	
Northwestern University HerStory Volunteer	2018

Society of Women Engineers (SWE)

2017

Career Day for Girls Volunteer

Northwestern Mentorship Opportunities for Research Engagement

2017

Mentor for high school students

References

Prof. Dr. Kurt Kremer

Director and Scientific Member at the Max Planck Institute for Polymer Research

Ackermannweg 10, 55128 Mainz, Germany

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Email: kremer@mpip-mainz.mpg.de

Prof. Dr. George C. Schatz

Morrison Professor of Chemistry; Professor of Chemical and Biological Engineering

Department of Chemistry

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Prof. Dr. Monica Olvera de la Cruz

Lawyer Taylor Professor of Materials Science and Engineering

Professor of Chemistry

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