Rasha Atwi

Computational Chemistry · Cheminformatics · Scientific Computing

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Education and Training

Stony Brook University — Stony Brook, NY
Ph.D. in Chemical Engineering, GPA: 4.0 — Sep 2018 - August 2024
Thesis: On exploring electrolyte solutions for next-generation batteries

Northeastern University — Boston, MA
M.S. in Chemical Engineering, GPA: 4.0 — Sep 2016 - Aug 2018
Thesis: A kinetic study of the formation of nitrogen heterocycles during HTL of micro-algae

American University of Beirut — Beirut, Lebanon
B.E. in Chemical Engineering, GPA: 3.7 (Distinction) — Sep 2012 - May 2016

Skills

Software	LAMMPS, Gaussian, VMD, Amber, Schrödinger Suites, OpenEye, RDKit, OpenBabel, Vortex, Spotfire
Programming	Python, Cython, MATLAB, Bash, Shell
Data Science & ML	NumPy, pandas, plotly, TensorFlow, Keras
Development Tools	Git, Jupyter, LATEX, Linux, NoSQL, HPC/Slurm

Industry Experience

Biogen — Cambridge, MA
Scientist — Sep 2024 - Present
- Developing a modular scientific workflow for building ultra-large small-molecule collections for ligand-based virtual screening, critical for early-stage drug discovery and hit identification.
- Optimizing workflow efficiency using advanced cheminformatics and high-performance computing techniques.
- Leading an external collaboration to advance computational chemistry capabilities and implement a GPU-accelerated virtual screening software that can rapidly screen 1 million compounds in 16 seconds.
- Supporting medicinal chemistry projects by assisting in SAR analysis and modeling to address data gaps and advance target-specific drug development.

Merck & Co. — Rahway, NJ
Computational and Structural Chemistry Intern — Jun 2023 - Aug 2023
- Investigated the reaction mechanism behind nitrosamine formation in drug products—a carcinogenic and genotoxic compound that caused FDA recalls.
- Built and validated a model utilizing physics-based and machine learning approaches to predict nitrosamine yield. The model streamlines risk assessments by identifying secondary amines with high risk of forming nitrosamines.

Biogen — Cambridge, MA
Computational Chemistry Co-op — Jan 2023 - May 2023
- Developed a user-friendly, GPU-accelerated 3D molecular alignment and shape comparison toolkit for virtual screening applications.
- Benchmarked the toolkit against ROCS, demonstrating comparable performance and robustness across multiple target classes, leading to its adoption by Biogen's medicinal chemistry department and significant reductions in annual licensing costs.

CF Technologies Inc. — Hyde Park, MA
Safety Consultant — Jan 2018 - May 2018
- Reviewed the HAZOP considerations of a pilot unit that extracts oil from brown grease using supercritical fluids.
- Developed a process flow diagram (PFD) and a piping and instrumentation diagram (P&ID) for the pilot unit.

Power Advocate (Part of Wood Mackenzie) — Boston, MA
Energy Business Analyst Co-op — Jul 2017 - Dec 2017
- Created cost models for specialty chemicals, equipment, and services used by the energy sector.
- Developed commodity forecasts, performed market analysis, and conducted research for publishing metals and chemicals foresights.

Software Development

ROSHAMBO

Main Developer & Maintainer — Jan 2023 - Present

A Python package for robust Gaussian molecular shape comparison.

GitHub repository: https://github.com/molecularinformatics/roshambo

MISPR: Materials Informatics for Structure Property Relationships

Main Developer & Maintainer — Sep 2018 - Present

An open-source Python package for automating materials science computations (DFT and MD simulations).

GitHub repository: https://github.com/molmd/mispr

MDPropTools

Main Developer & Maintainer — Sep 2018 - Present

An open-source Python package for statistical analysis of MD trajectories and output files to compute properties of liquid solutions.

GitHub repository: https://github.com/molmd/mdproptools

Academic Research

Stony Brook University — Stony Brook, NY

Graduate Research Assistant — 2018 - 2024

- Explored structural and dynamical properties of electrolytes and electrode-electrolyte interfaces in next-generation batteries using DFT and MD simulations.
- Built computational databases for high-throughput screening of electrolytes for Li-S batteries.
- Developed new computational methods for predicting spectroscopic signatures in liquid solutions. The methods address some of the most challenging aspects of computational spectroscopy - equilibrium conformers and solvation effects.
- Collaborated with a computer science team to fine-tune a BERT-based NLP model for extracting electrolyte properties from scholarly text.
- Wrote open-source software packages for automating high-throughput multi-scale simulations on supercomputers.

Northeastern University — Boston, MA

Graduate Research Assistant — 2016 - 2018

Developed a kinetics model using *ab-initio* thermodynamic simulations for the formation of nitrogen heterocycles during hydrothermal liquefaction of micro-algae.

Centre for the Theory and Application of Catalysis, Queen's University Belfast — Belfast, UK

Visiting Research Associate — 2015

Synthesized, characterized, and tested heterogeneous catalysts for Fischer Tropsch reaction and operated and controlled chemical rigs.

American University of Beirut — Beirut Lebanon

Undergraduate Research Assistant — 2013 - 2014

Identified pharmaceutical compounds present in the Lebanese water bodies based on physic-chemical properties and prescription data.

Honors and Awards

Academic Excellence Award, Stony Brook University — 2024

Graduate Service Award, Stony Brook University — 2024

Early Career Group Best Poster Award, Battery+Energy Storage Conference, Argonne National Lab — 2023

IACS Junior Researcher Award, Stony Brook University — 2021 - 2024

"Given to continuing PhD graduate students who are recognized as outstanding junior researchers by institute faculty or affiliates."

Dean's Fellowship, Tufts University — 2018 - 2020

"To recognize and recruit exceptional incoming doctoral students."

College of Engineering Top GPA Award, Northeastern University — 2019

Outstanding Seminar Award, Northeastern University — 2018

Best Student Poster Award, American University of Beirut 2016

Dean's Honor List, American University of Beirut 2016
"Ranked in the top 10% of the class."

Teaching and Research Mentoring

Workshop Helper, Software Carpentry 2023
Assisted learners one-on-one with software installation, understanding specific lines of code, and other aspects of the learning process related to bash, Git version control, and programming in Python. Link.

MISPR Workshop Instructor, Stony Brook University Jul 2022
Organized and ran MISPR hands-on workshop at iACS to introduce high-school students to materials informatics techniques. Link.

Research Mentor, Stony Brook University / Tufts University 2019 - 2022
- Mentored high-school and undergraduate students on projects related to force field database development and electrolyte property predictions.
- Introduced students to computational chemistry techniques, including DFT, and provided hands-on experience in programming to automate tasks and analyze data effectively.

Teaching Assistant, Tufts University 2018 - 2020
- Courses: Transport phenomena (CHBE-0022), Advanced thermodynamics (CHBE-0203).
- Held office hours and reviewed and graded homework problems, reports, and exams.
- Led recitation and tutorial sessions to review concepts and work through practice problems.

Professional and Community Activities

Academic Peer Reviewer, WoS ResearcherID: IXN-5252-2023. 2023 - Present
Conferences: ICLR-ml4materials (2), NeurIPS-AI4Mat (3). ICML-AI4Mat (1), Journals: J. Open Source Softw. (2)

Energy and Fuels Committee Member, American Chemical Society 2023 - Present
Develop a plan to increase membership of students, industry, and international members in the division.

Volunteer in the Fellowship Program, Women in High-Performance Computing 2023 - Present
Review travel fellowship applications for the supercomputing conference (SC) held each year.

Mentor at the Intercultural Conversation Program, Tufts University 2019
Helped international graduate students adjust to life in the U.S. and build confidence in their conversational English through weekly one-on-one meetings.

Publications

† = equal contribution | Google Scholar | ORCID: 0000-0001-8122-7335

11. Mathison, R., **Atwi, R.**, et al. (2025). "Molecular processes that control adiponitrile electrosynthesis in near-electrode microenvironments". JACS, 0002-7863.
10. **Atwi, R.**, Gribble, D., et al. (2024). "Knowledge-driven design of fluorinated ether electrolytes via a multi-model approach". Preprint.
9. **Atwi, R.**, Wang, Y., et al. (2024). "ROSHAMBO: Open-source molecular alignment and 3D similarity scoring". Journal of Chemical Information and Modeling, 64(21), 8098-8104.
8. Chen, Y.†, **Atwi, R.†**, Nguyen, D.T.†, et al. (2024). "From bulk to interface: solvent exchange dynamics and their role in ion transport and the interfacial model of rechargeable magnesium batteries". JACS, 146, 19, 12984–12999.
7. **Atwi, R.** & Rajput, N. N. (2023). "Guiding maps of solvent classes for lithium-sulfur batteries via a computational data-driven approach". Patterns, 4(9).
6. Li, Z., Rao, H., **Atwi, R.**, et al. (2023). "Non-polar ether-based electrolyte solutions for stable high-voltage non-aqueous lithium metal batteries". Nature Communications, 14, 868.
5. **Atwi, R.**, Bliss, M., et al. (2022). "MISPR: An open-source package for high-throughput multiscale molecular simulations". Scientific Reports, 12, 15760.

4. **Atwi, R.**, Chen, Y., et al. (2022). "An automated framework for high-throughput predictions of NMR chemical shifts within liquid solutions". Nature Computational Science, 2(2), 112-122.
3. LeClerc, H. O., **Atwi, R.**, et al. (2022). "Elucidating the role of reactive nitrogen intermediates in hetero-cyclization during hydrothermal liquefaction of food waste". Green Chemistry, 24(13), 5125-5141.
2. Chen, Y., **Atwi, R.**, et al. (2021). "Role of a multivalent ion–solvent interaction on restricted Mg^{2+} diffusion in dimethoxyethane electrolytes". The Journal of Physical Chemistry B, 125(45), 12574-12583.
1. Blanco, D. E., **Atwi, R.**, et al. (2020). "Effect of electrolyte cations on organic electrosynthesis: the case of adiponitrile electrochemical production". Journal of The Electrochemical Society, 167(15), 155526.

Posters and Presentations

17. **Atwi, R.** & Rajput, N. N. (Fall 2023). "An automated multi-scale NMR framework helps understand solvent exchange dynamics in multivalent batteries". MRS Meeting. Oral Presentation.
16. **Atwi, R.** & Rajput, N. N. (Fall 2023). "Guiding maps of solvents for lithium-sulfur batteries via a computational data-driven approach". 5th Battery and Energy Storage Conference (Argonne National Laboratory). Poster Presentation.
15. **Atwi, R.** & Rajput, N. N. (Fall 2022). "Data-driven prediction of structure and dynamic features of Li-S electrolytes with an automated multi-scale computational infrastructure". MRS Meeting. Oral Presentation.
14. **Atwi, R.** & Rajput, N. N. (Fall 2022). "Data-driven investigation of solvents for lithium-sulfur battery liquid electrolytes". ACS Meeting. Oral Presentation.
13. **Atwi, R.** & Rajput, N. N. (Fall 2022). "Towards accurate predictions of NMR chemical shifts in liquid solutions". ACS Meeting. Oral Presentation.
12. **Atwi, R.**, Bliss, M. M., & Rajput N. N. (Summer 2022). "MISPR: A novel framework for high-throughput multi-scale modelling of complex liquid solutions". FOMMS: Molecular Modeling and the Data Revolution Conference. Poster Presentation.
11. **Atwi, R.** & Rajput, N. N. (Spring 2022). "Tailoring atomistic interactions in Li-S battery via a computational multi-scale data-driven approach". 241st ECS Meeting. Oral Presentation.
10. **Atwi, R.** (Spring 2022). "Towards next generation batteries via high-throughput modelling of electrolytes". IACS Brown Bag Lunch. Oral Presentation.
9. **Atwi, R.** (Fall 2022). "Tailoring atomistic interactions in Li-S battery via a computational multi-scale data-driven approach". IACS Student Seminar. Oral Presentation.
8. Rajput, N. N. & **Atwi, R.**. (Spring 2021). "Designing optimal electrolytes and interfaces in Li-S batteries". 239th ECS Meeting. Invited Oral Presentation.
7. Rajput, N. N. **Atwi, R.**, & Bliss, M. (Spring 2021). "A multi-scale infrastructure for automating materials science computations". 239th ECS Meeting. Invited Oral Presentation.
6. **Atwi, R.** & Rajput, N. N. (Spring 2021). "Effects of functionalized cathode and electrolyte composition on structure and dissolution of polysulfide species in Li-S batteries". MRS Meeting. Oral Presentation.
5. **Atwi, R.** & Rajput, N. N. (Fall 2020). "Tailoring atomistic interactions in Li-S battery via a computational multi-scale-data-driven approach". MRS Meeting. Oral Presentation.
4. **Atwi, R.**, Bliss, M. M., & Rajput N. N. (Fall 2020). "A high-throughput multi-scale infrastructure for automating materials science computations". MRS Meeting. Oral Presentation.
3. Timko, M. T., West, R. H., & **Atwi, R.** (2019). "Understanding formation of nitrogen heterocycles during catalytic hydrothermal liquefaction". AIChE Annual Meeting. Oral Presentation.
2. **Atwi, R.**, Timko, M. T., & West, R. H. (Fall 2018). "Investigating reaction pathways for the formation of nitrogen heterocycles during hydrothermal liquefaction of microalgae". ACS Meeting.
1. **Atwi, R.** & West, R. H. (Summer 2017). "Understanding the source of undesired nitrogen heterocycles in biofuel made by hydrothermal liquefaction of micro-algae". New England Energy Research Forum. Poster Presentation.