Omri David Abarbanel, Ph.D.

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Education

University of Pittsburgh — Pennsylvania, USA
PhD - Computational Chemistry — *August 2024*
Thesis: *Combining Quantum Mechanical Calculations with Machine Learning and Genetic Algorithms* for the Design of Better Materials.

City University of New York - Hunter College — New York, USA
B.Sc. - Chemistry; Special Honors Curriculum — *May 2017*
Thomas Hunter Honors Student. *Magna Cum Laude.*
Research Project: *Green synthesis and characterization of zinc oxide nanoparticles.*

Skills

- **Programming:** Python, Bash. SQL, LaTeX
- **Data Science:** Pandas, NumPy, SciPy
- **Machine Learning:** Scikit-learn, PyTorch, HuggingFace
- **Cheminformatics:** RDKit, OpenBabel, ORCA, Gaussian, xTB
- **Visualization:** Matplotlib, Seaborn, Plotly, Bokeh
- **Tools:** Git, Slurm, HTC, Jupyter
- **Soft Skills:** Team Leadership, Problem Solving
- **Spoken Languages:** Hebrew: Native, English: Fluent

Experience

National Energy Technology Laboratory
ORISE Postdoctoral Fellow | *September 2024 - Current*

- **Visualization Tools:** Building interactive visualizations of emissions data in Python, using Plotly, to help identify emission sources.
- **Large Language Models:** Working with an interdisciplinary team to build large language models (LLM) to predict methane emissions and help with mitigation, achieving over 80% accuracy.

University of Pittsburgh
Graduate Student Researcher — *August 2018 – August 2024*

- **Machine Learning for Molecular Property Prediction:** Using different machine learning models such as random forest, gradient-boosted trees, deep neural networks, graph neural networks and message-passing neural networks, as well as active learning and transfer learning, to predict molecular properties like polymers' reorganization energy and micro-pK_a of drug-like molecules.
- **Genetic Algorithms for Molecular Property Optimization:** Using genetic algorithms to accelerate the search for novel materials with various properties.
- **Quantum Mechanical Calculations:** Using quantum mechanical calculations with machine learning and genetic algorithms to find better materials. Experience in using popular quantum calculation programs such as ORCA and Gaussian.
- **Data Engineering:** Feature engineering using data from publicly available datasets, as well as generating custom data for machine learning applications.
- **Research Communication**: Successfully presented research results to a multidisciplinary audience in multiple conferences, receiving accolades and recognition.
- **Open-Source Contributions**: Added new functionalities to the cclib 2.0 Python package, which is used by over 5,000 users.
- **Peer Reviewer:** For the Journal of Applied Physics.
- **Teaching and Tutoring:** For general, organic, and physical chemistry undergraduate-level labs and classes

City University of New York - Advanced Science Research Center
Research Intern — *May 2017 - July 2018*

- ***Research Project:*** *Used Second Harmonics Generation imaging to characterize peptide self-assemblies.*
- ***Microfluidic Devices:*** *Designed and created microfluidic devices to control the growth of peptide self-assemblies.*

Israel Ministry of Tourism
IT, Social & Digital Media Director — *November 2011 - April 2016*

- **IT:** Managed the computer systems for 50 end users in 5 offices across the US and Canada.
- **Social Media:** Managed the Tourism office's Facebook, Twitter and YouTube accounts targeted at the North American market. Revitalized social networks presence and increased engagement with potential tourists by 600%. Oversaw three social media campaigns that increased the number of followers by more than half a million.
- **Digital Media:** Managed the Tourism office's website, including updating content and images.

RSA

Software as a Service - Tier 1 *November 2010 - September 2011*

- **System Monitoring:** Supported and monitored systems used for cyber security for US and European banks.
- **Team Schedule:** Managed the teamwork schedule to accommodate every team member's needs.

Israel Defense Force

Network Administrator *October 2007 - April 2010*

- **Team Manager**: Managed a team of 5 people. The role included teaching new members, managing the team schedule, and overall management.
- **Network Administration:** Managed the computer network for 300 end-users, including general fixing, upgrading, and monitoring of the system.
- **Reporting:** Wrote SQL-like code to generate reports for all departments at the center.

Publications

Machine learning to accelerate screening for Marcus reorganization energies

Abarbanel, Omri D., and Hutchison, Geoffrey R.

The Journal of Chemical Physics, vol. 155, pp. 054106, 2021

- Used machine learning algorithms as a surrogate to quantum mechanical computations for the discovery of conductive and semi-conductive organic copolymers with small reorganization energies.
- Developed an optimized molecular representation for machine learning that included quantum mechanical features and tested various models for their predictive performance.

Strategies for Computer-Aided Discovery of Novel Open-Shell Polymers

Abarbanel, Omri D., Rozon, Julisa, and Hutchison, Geoffrey R.

The Journal of Physical Chemistry Letters, vol. 13, pp. 2158-2164, 2022

- Performed a computational study to find a predictive molecular quantity to aid in the discovery of conjugated organic copolymers with stable triplet ground state.
- Discovered a faster semi-empirical method that correlates with the slower density-functional theory method. This can accelerate the search for new triplet ground-state copolymers.

Using Genetic Algorithms to Discover Novel Ground-State Triplet Conjugated Polymers

Abarbanel, Omri D., and Hutchison, Geoffrey R.

Phys. Chem. Chem. Phys., 2023, 25, 11278-11285.

- Used a genetic algorithm in conjunction with a semi-empirical method to accelerate the search for novel conjugated co-polymers with a stable triplet ground-state.
- Found more than 1400 polymer candidates and analyzed the most common monomers to obtain information on the structural and electronic properties that influence the stability of the triplet ground state.

QupKake: Integrating Machine Learning and Quantum Chemistry for micro-pK_a Predictions

Abarbanel, Omri D., and Hutchison, Geoffrey R.

Journal of Chemical Theory and Computation 2024 20 (15), 6946-6956

- Used graph neural networks to predict micro-pK_a values for small drug-like organic molecules.
- Developed a model that improved current state-of-the-art micro-pK_a predictions and decreased the error by 30% by combining semi-empirical quantum mechanical features and using a transfer learning pipeline model training.

Honors and Awards

RSA Team Award - April 2011:

- Managed the shift schedule on time when there was a staff shortage and scheduling conflicts.
- Volunteered to do multiple double shifts to keep the 24/7 operations unaffected.

IDF Excellence in Service Award - May 2010:

- Built a system to streamline the recruitment center workflow that saved money on unrecovered items.
- Built a system for a new department, saving time and resources, and had a quick turnaround for changes or additions.
- Efficiently and politely managed the IT department for 300 end-users in the recruitment center.