# Omri David Abarbanel

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## EDUCATION

**University of Pittsburgh** — Pennsylvania, USA
*PhD - Computational Chemistry* — *August 2018 - May 2023 (Expected)*
**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* — *January 2013 - May 2017*
**Thomas Hunter Honors Student**. *Magna Cum Laude.*
**Research Project:** *Green synthesis and characterization of zinc-oxide nanoparticles.*

## SKILLS

- **Languages**: Python, Bash, SQL, LaTeX
- **Frameworks**: Scikit, Pytorch, TensorFlow, Keras
- **Data Wrengling**: Pandas, NumPy
- **Visualization**: Matplotlib, Seaborn, Plotly
- **Tools**: Git, Slurm, HTCondor, Jupyter
- **Soft Skills**: Team Leadership, Technical Writing

## EXPERIENCE

**University of Pittsburgh**
*PhD Candidate* — *August 2018 - Present*
- **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 more, to predict molecular properties like reorganization energy and micro-pKa.
- **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.

**University of Pittsburgh**
*Teaching Assistant* — *August 2018 - Present*
- **Teaching**: Tought General, organic, and physical chemistry undergraduate-level labs.
- **Tutoring**: Tutored general and organic chemistry to individuals and groups.

**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.

**City University of New York - Hunter College**
*Teaching Assistant* — *May 2017 - July 2018*
- **Teaching**: Tought General and organic chemistry undergraduate-level labs.
- **Tutoring**: Tutored general and organic chemistry to individuals and groups.

**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 the social media presence and greatly increased engagement with potential tourists. Oversaw three social media campaigns that increased the number of followers by over half-a-million.
- **Digital Media**: Managed the Tourism office's website, including updating content and images.
- **Information Center**: Answered tourists' questions about visiting Israel.

**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 team work schedule to accomodate every team member's needs.

**Israel Defence Force**

*Recruitment Center - Network Administrator*                    *October 2007 - April 2010*

- **Team Manager**: Managed a team of 5 people. Role included teaching new members, managing team schedule, and overall management.
- **Network Adminitration**: Managed the compoter network for 300 end-users, including general fixing, upgrading, and monitoring of the system.
- **Reporting**: Wrote SQL-like code to generate reports for all the departments in 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 co-polymers with small reorganization energies.
- Developed an optimized molecular representation for machine learning that included quantum mechanical features, and tested various models for their predictive performances.

**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 co-polymers with a stable triplet ground-state.
- Discovered a faster semi-empirical method which correlates with the slower density-functional theory method. This can accelerate the search for new triplet ground-state co-polymers.

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

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

*Chemical Science (in review). ChemRxiv.*

- Used a genetic algorithm in conjuction 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 elecronic properties that influence the stability of the triplet ground-state.

## OTHER PROJECTS

**xTB parsing integration for the *cclib* package**:

- Adding support for parsing xTB-generated output files to the *cclib* python package (work in progress).

## HONORS AND AWARDS

- **RSA Team Award**: For helping the team continue to operate during a complicated time - April 2011
- **IDF Excelence in Service Award**: For my above-and-beyond service in the IDF - May, 2010

## VOLUNTEER EXPERIENCE

**ACS Colloids Symposium - July 2017**

- Managed the computer system for the whole symposium.
- Gave support and solved problems quickly to not disturb the flow of the presentations.
- The organizers highly appreciated my knowledge and hard work during the symposium.

## HOBBIES

- Baking & Cooking
- Biking
- 3D Printing
- Electronics (Arduino, Rasspbery-Pi)
- Musical Theather