Dr David Furman, PhD

Contact Information

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MANOR Advanced Technologies Division
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Research Interests

Computational Chemical Science: Multiscale Simulation, Reactive Molecular Dynamics, Reactivity in Extreme Conditions, Numerical Methods

Current Appointments

Research Scientist, Simulation Group, MANOR Division, RAFAEL Ltd.
Feb. 2022 - present

Education

The Hebrew University, Jerusalem, Israel

PhD., Theoretical Chemistry, Dec. 2017

- Thesis Topic: *Computational Studies of Energetic Materials from an Atomistic Perspective*
- Advisers: Prof. R. Kosloff and Prof. Y. Zeiri

MSc., Theoretical Chemistry, Aug. 2013

- Thesis Topic: No thesis, Direct PhD Track
- Advisers: Prof. R. Kosloff and Prof. Y. Zeiri

Ben Gurion University, Be'er-Sheva, Israel

BSc., Chemistry (*magna cum laude*), Aug. 2009

Grants

Awarded

[5] Principal Investigator, "Deep Learning Solid Propellant Mechanical Properties", AI start-up grant, RAFAEL Ltd., 01 July., 2022 to 01 July., 2024 (NIS 600,000).

[4] Principal Investigator, "Unraveling solvent effects on emergence of simple peptides: How likely is life on Titan?", EPSRC HPC Access grant, HPCSSUP-27483, 01 Feb., 2020 to 01 Feb., 2021 (£68,000).

[3] Co-PI (with Prof. D. J. Wales), "Accelerated Discovery of Molecular Mechanisms on Prebiotic Earth", EPSRC Tier-2 capital grant, EP/P020259/1, 01 Feb., 2019 to 01 Feb., 2020 (£215,000).

[2] Co-PI (with Prof. M. Caspary-Toroker), "HPC for Computational Modeling", PAZY-IAEA 4880520, Jan. 1, 2017 to Jun. 30, 2018 ($70,131).

[1] Co-PI (with Prof. M. Caspary-Toroker), "Theoretical Modeling of Nickel Oxide Fuel Cells", PAZY-IAEA 14580239, Jan. 1, 2016 to Jun. 30, 2019 ($91,234).

Advising and Mentoring

Postdoctoral Scholars

- **Dr Kapil Dhaka**, 2017-2019, Materials Science and Engineering, Technion Israel Institute of Technology
  Co-advised by: Maytal Caspary-Toroker

Graduate Students

- **Mr Evgeny Moerman**, 2018, MSc candidate, Chemistry, University of Cambridge
  Co-advised by: David J. Wales
- **Mr Yuval Elbaz**, 2017-2019, PhD candidate, Physics and Materials Science and Engineering, Technion Israel Institute of Technology
  Co-advised by: Maytal Caspary-Toroker
- **Mrs Vicky Fidelsky**, 2016-2017, MSc candidate, Materials Science and Engineering, Technion Israel Institute of Technology
  Co-advised by: Maytal Caspary-Toroker

Research Staff

- **Dr Yuri Khodorkovsky**, 2016-2018, Computational Chemistry Group, NRCN
- **Dr Erez Boukobza**, 2016-2018, Computational Chemistry Group, NRCN
- **Mr Doron Haviv**, 2016-2018, Chemical Engineering Division, NRCN

Teaching Experience

University of Cambridge, Cambridge, UK

Senior Demonstrator **Academic Year 2019/2020**

- Part II Practicals, Theoretical Chemistry (undergraduate course)

Negev - Nuclear Research Centre, IL

Instructor **2016-2018**

- Computational Chemistry in Chemical Process Engineering (professional development)

Ben Gurion University of the Negev, Be'er-Sheva, IL

Private Groups Lecturer **Academic Year 2013/2014**

- Quantum Chemistry I (undergraduate course)

Yeruham Center for Education, Yeruham, IL

Chemistry Teacher **Academic Year 2012/2013**

- Chemistry (high school level)

Professional Service

Committees

- Member of the Governing Body, Darwin College, University of Cambridge, Sept. 2021 - Sept. 2022

Journals Referee

- *Journal of the American Chemical Society*
- *Journal of Chemical Theory and Computation*
- *Journal of Physical Chemistry C*
- *Journal of Physical Chemistry Letters*
- *ACS Omega*
- *Frontiers in Chemical Science and Engineering*
- *Molecular Physics*
- *ACS Applied Materials*
- *Computational and Theoretical Chemistry*
- *Physical Chemistry Chemical Physics*

Professional Experience

University of Cambridge, Cambridge, UK

Herchel Smith Research Fellow **Sept. 2018 - 2021**

- Energy Landscape Theory for reactive phenomena, reactive force fields, global optimisation, enhanced sampling, multi-scale modeling, software development. Applications to chemical reaction networks, catalysis and prebiotic chemistry. Host: Prof. D. J. Wales (Chemistry Department).

Shimon Peres Negev Nuclear Research Center, Be'er-Sheva, IL

Computational Chemistry Group Leader **Aug. 2015 to Aug. 2018**

- Chief responsibility for development and application of computational methods to predict materials properties from first principles, optimal control of chemical engineering processes, modeling and data analysis.
- Supervision and mentoring of process engineers, staff scientists and technical staff.

Staff Scientist **Jun. 2013 to Aug. 2015**

- Development and application of computational methods to predict materials properties from first principles, optimal control of chemical engineering processes, modeling and data analysis.

Penn. State University, State College, PA

Visiting Scholar **Sept. 2012**

- Development of ReaxFF reactive force fields for azides

Professional Memberships

Academic societies

- American Chemical Society (2015–present)
- Royal Society of Chemistry (2018–present)
- American Physical Society (2015–present)

Awards

Darwin Research Fellowship

- Independent research fellowship at Darwin College, University of Cambridge, 2020–2023

Herchel Smith Research Fellowship

- Independent research fellowship at the University of Cambridge, 2018–2021

Aharon Katzir Research Fellowship

- A 6-year research fellowship at NRCN, 2016–2022

Direct PhD Track, Hebrew University of Jerusalem

- Qualification to the direct to PhD track for excellent 1st year Msc students, 2014

"100 Club" award of the Academic Reserve of the IDF

- "100 Club" award for excellent academic achievements, 2014

Zlotowski admission award, Ben-Gurion University

- Zlotowski admission award for excellent academic achievements, 2007