Renana Gershoni Poranne

Schulich Faculty of Chemistry – Technion – Haifa, Israel
rporanne@technion.ac.il
n.ethz.ch/~rporanne/

Professional Experience

Last Updated: August 2022

since 2021 **Assistant Professor** Technion – Israel Institute of Technology
since 2019 **Branco Weiss Fellow** ETH Zürich, Technion – Israel Institute of Technology
2017-2021 **Group Leader / "Habilitandin"** within the group of Prof. Peter Chen, ETH Zürich
2015-2017 **Postdoctoral Researcher** with Prof. Peter Chen, ETH Zürich

Education

2010-2015 **Ph.D.** — Schulich Faculty of Chemistry, Technion, Israel.
Thesis: *Aromatic Systems*
Advisor: Prof. Amnon Stanger

2007-2010 **M.Sc.** *(Summa cum Laude)* — Schulich Faculty of Chemistry, Technion, Israel.
Thesis: *Novel Corannulene-Aryl Ethers as Pentagonal Building Blocks for Superstructures*
Advisor: Prof. Ehud Keinan

2004-2007 **B.Sc.** *(Summa cum Laude)* — Schulich Faculty of Chemistry, Technion, Israel.
Major: *Molecular Biochemistry*

Fellowships

2022 Alon Scholarship – Integration of Outstanding Faculty
2021 Horev Fellowship – Leaders in Science and Technology
2019 Branco Weiss Fellowship – Society in Science
2016-2018 The VATAT Fellowship for Excellent Female Post-Doctoral Scholars
2012-2014 The Schulich Fellowship for Excellence in Graduate Studies – Ph.D.
2007-2009 The Schulich Fellowship for Excellence in Graduate Studies – M.Sc.

Honors and Awards

2021 Golden Owl Award for Excellence in Teaching at ETH Zurich
2018 Junior Scientist Participation award to attend the '53rd Bürgenstock Conference'
2017 Poster Award at GRC Physical Organic Chemistry; Poster chosen for talk
2015 The Weissman and Jacknow Prize for Continued Excellence in Teaching
2014 The Schulich Prize for Excellence in Teaching
2014 Vivian Konigsberg Award for Continued Excellence in Teaching
2013 Selected to be a participant in the 63rd Lindau Nobel Laureates Meeting (Chemistry)
2013 Selected to be a participant in the 1st Global Young Scientists Summit, Singapore
2013 Sandor Szego Award for Excellence in Teaching
2012 The Schulich Prize for Excellence in Teaching
2010 Sandor Szego Award for Excellence in Teaching
2009 Sandor Szego Award for Excellence in Teaching

2009 The Schulich Prize for Excellence in Teaching

2008-2009 Sharett Foundation Scholarship for Excellence in Music – Singing

2008 Vivian Konigsberg Award for Excellence in Teaching

2007 Schulich Prize for Excellence in Undergraduate Studies

2007 Knesset (Israeli Parliament) Award for Excellent Undergraduate Students

2007-2008 Sharett Foundation Scholarship for Excellence in Music – Singing *(with distinction)*

2004-2007 President of the Technion's Award for Excellence in Studies, 5 semesters *(top 3%)*

Supervision of Students

Ph.D. Theses

current Shany Erez (Technion)

Revealing Structure-Property Relationships in peri-Condensed Polybenzenoid Hydrocarbons using Deep-Learning

current Alexandra Wahab (ETH Zürich)

Inverse Design of Polycyclic Aromatic Hydrocarbons

M.Sc. Theses

current Eduardo Mayo (Technion)

Development of Novel Text-based Representations for Polycyclic Aromatic Systems

2019-2020 Stefan Feusi (ETH Zürich)

On the Origin of Additive Aromaticity: Current Density and Molecular Orbital Analyses

2016-2017 Eno Paenurk (ETH Zürich)

Theoretical Study of Metallophilic Interaction in d^8-d^{10} Complexes

M.Sc. Semester Projects

2021 Dominic Egger (ETH Zürich)

Jahn-Teller Distortion in Triplet-State Polybenzenoid Hydrocarbons

2020 Lara Pfuderer (ETH Zürich)

Correlations between xTB and B3LYP for Enabling High Throughput Data Generation

2019 Greta Markert (ETH Zürich)

NICS-XY-Scans of Triplet-State Polycyclic Aromatic Hydrocarbons

2019 Stefan Feusi (ETH Zürich)

PREDI-XY: Automated Generation of NICS-XY Scans with Additivity

2018 Patrick Finkelstein (ETH Zürich)

Additive Aromaticity: The Heteroatom Case

B.Sc. Semester Projects

current Sahar Sagy (Technion)

Machine Learning the Relationship between Aromatic Indices

Teaching Experience – Summarized

As Lecturer at Technion

2022 Lecturer – *Molecular Orbitals in Organic Chemistry*

As Lecturer at ETH Zurich

2018-2021 Lecturer – *Organic Chemistry IV: Physical Organic Chemistry*

As Teaching Assistant at Technion

2009-2015 Senior Teaching Assistant – *Principles of Chemistry A; Principles of Chemistry B; Organic Chemistry Expanded 1; Organic Chemistry Expanded 2; Structure Determination by Physical Methods*

2008-2009 Teaching Assistant and Lab Instructor – *Principles of Chemistry A; Principles of Chemistry B*

Oral Presentations at International Conferences

13. **(Upcoming – Invited Talk)** From Electronic Structure of Organics to Organic Electronics
Gordon Research Conference Physical Organic Chemistry — Holderness, NH, USA **June, 2023**

12. **(Upcoming – Invited Talk)** Exploring the Chemical Space of Polybenzenoid Hydrocarbons with Interpretable Models
The 3rd "Carbon" Fusion Conference — Tulum, Mexico **May, 2023**

11. **(Upcoming – Invited Talk)** Text-Based Representation of Polybenzenoid Hydrocarbons Reveals Structure-Property Relationships in the Excited State
The 2nd International Conference on Excited State Aromaticity and Antiaromaticity — Hawaii, USA **December, 2022**

10. **(Upcoming – Invited Talk)** Revealing Structure-Property Relationships in Polybenzenoid Hydrocarbons using Interpretable Machine- and Deep-Learning Methods
The MAGIC Workshop — Cambridge, UK **September, 2022**

9. **(Upcoming)** Breaking it Down: Characterization of Polybenzenoid Hydrocarbons Using Their Subunits
The Batsheva de Rothschild Seminar on Strong Bond Activation — Ein Gedi, Israel **October, 2022**

8. **(Invited Talk)** Predicting Molecular Properties of Polybenzenoid Hydrocarbons Using Their Subunits
WATOC, the 12th Triennial Congress — Vancouver, Canada **2022**

7. **(Invited Talk)** Patterns in Aromaticity of Triplet State Polycyclic Aromatic Hydrocarbons
International Conference on Excited State Aromaticity and Antiaromaticity — Sigtuna, Sweden **2019**

6. **(Invited Talk)** Predictive Aromaticity and Predicting Aromaticity
Aromaticity 2018 — Riviera Maya, Mexico **2018**

5. The Predictive Power of Aromaticity
International Symposium on Reactive Intermediates and Unusual Molecules (ISRIUM) — M. Verita, Switzerland **2018**

4. Additive Aromaticity in One, Two, and Three Dimensions
IUPAC International Conference on Physical Organic Chemistry (ICPOC) — Faro, Portugal **2018**

3. **(Poster Prize Talk)** Additivity with NICS-XY-Scans
Gordon Research Conference on Physical Organic Chemistry — Holderness, NH, USA **2017**

2. The NICS-XY-Scan: Identification of Global and Local Ring Currents in Polycyclic Systems
Schulich Graduate Students Symposium — Technion, Haifa, Israel **2014**

1. Is There a Correlation Between the Induced Ring Currents and the Aromatic Stabilization Energies of the [N]Phenylenes?
Lise Meitner – Minerva Center for Computational Chemistry Symposium — Hebrew University, Jerusalem, Israel **2012**

Selected Poster Presentations

This list details poster presentations from the past five years only.

6. Patterns in Aromaticity of Triplet Polycylic Aromatic Hydrocarbons
Gordon Research Conference on Physical Organic Chemistry — Holderness, NH, USA **2019**

5. PREDI-XY: An Automated System for Generation of NICS-XY Scans with Additivity
Gordon Research Conference on Physical Organic Chemistry — Holderness, NH, USA **2019**

4. Additive Aromaticity: The Heteroatom Case
International Symposium on Reactive Intermediates and Unusual Molecules — Monte Verita, Switzerland **2018**

3. Additive Aromaticity in One, Two, and Three Dimensions
53rd Bürgenstock Conference — Brunnen, Switzerland **2018**

2. Additivity with NICS-XY-Scans — *poster award; chosen for short talk*
Gordon Research Conference on Physical Organic Chemistry — Holderness, NH, USA **2017**

1. The C-N^+ Bonds in Amine and Ammonium Compounds are Charge-Shift Bonds
SPP 1807 Fall Meeting — Köln, Germany **2016**

Recent Publications in Peer-Reviewed Journals

This list details recent selected publications only. For a complete list of publications, please download the corresponding file here.
Note: * denotes corresponding author.

11. Alexandra Wahab, Lara Pfuderer, Eno Paenurk, and Renana Gershoni-Poranne*
The COMPAS Project: A Computational Database of Polycyclic Aromatic Systems. Phase 1: cata-Condensed Polybenzenoid Hydrocarbons
Journal of Chemical Information and Modeling, **2022**, *62*, 3704.
Selected for a *Front Cover*

10. Zheng Zhou, Dominic T. Egger, Chaowei Hu, Matthew Pennachio, Zheng Wei, Rahul K. Kawade, Ökten Üngör, Renana Gershoni-Poranne*, Marina A. Petrukhina*, and Igor V. Alabugin*
Localized Antiaromaticity Hot-spot Drives Reductive Dehydrogenative Cyclizations in Bis- and Mono-Helicenes
Journal of the American Chemical Society, **2022**, *144*, 12321
Selected for a *Front Cover*

9. Eno Paenurk* and Renana Gershoni-Poranne*
Simple and Efficient Visualization of Aromaticity: Bond Currents Calculated from NICS Values
Physical Chemistry Chemical Physics, **2022**, *24*, 8631.
Selected for a *Front Cover*

8. Renana Gershoni-Poranne* and Amnon Stanger*
Chapter 4: NICS – Nucleus Independent Chemical Shifts.
in Aromaticity: Modern Computational Methods and Applications, **2021**
Edited by I. Fernandez.

7. Greta Markert, Eno Paenurk, and Renana Gershoni-Poranne*
Prediction of Spin Density, Baird-Antiaromaticity, and Singlet-Triplet Energy Gap in Triplet-State Polybenzenoid Systems from Simple Structural Motifs
Chemistry - A European Journal, **2021**, *27*, 6923.
Selected for a *Cover Feature*

6. Eno Paenurk, Stefan Feusi, and Renana Gershoni-Poranne*
Predicting bond-currents in polybenzenoid hydrocarbons with an additivity scheme
Journal of Chemical Physics, **2021**, *154*, 024110.
Invited contribution for the *Issue Honoring Women in Chemical Physics and Physical Chemistry*

5. Alexandra Wahab, Felix Fleckenstein, Stefan Feusi, and Renana Gershoni-Poranne*
Predi-XY: A Python program for automated generation of NICS-XY-Scans based on an Additivity Scheme
Electronic Structure, **2020**, *2*, 047002.
Invited contribution for the *Emerging Leaders* issue

4. Z. Zhou, R. K. Kawade, Z. Wei, F. Kuriakose, Ö. Üngor, M. Jo, M. Shatruk, R. Gershoni-Poranne,* M. A. Petrukhina,* and I. V. Alabugin*
Negative charge as a lens for concentating antiaromaticity: using pentagonal "defect" and helicene strain for cyclizations
Angewandte Chemie Int. Ed., **2020**, *59*, 1256-1262.

3. P. Finkelstein and R. Gershoni-Poranne*
An Additivity Scheme for Aromaticity: The Heteroatom Case
ChemPhysChem **2019**, *20*, 1508-1520.

2. R. Gershoni-Poranne,* A. P. Rahalkar, and A. Stanger*
The Predictive Power of Aromaticity: Quantitative Correlation between Aromaticity and Ionization Potentials and HOMO-LUMO Gaps in Oligomers of Benzene, Pyrrole, Furan, and Thiophene
Physical Chemistry Chemical Physics **2018**, *20*, 14808-14817.

1. R. Gershoni-Poranne*
Piecing it Together: An Additivity Scheme for Aromaticity using NICS-XY-Scans
Chemistry – A European Journal **2018**, *24*, 4165-4172.

Academic Contributions

Reviewer for:

- *Nature Chemistry*
- *Journal of the American Chemical Society*
- *Chemical Science*
- *Angewandte Chemie*
- *Chemistry - a European Journal*
- *ChemistryOpen*
- *Israel Journal of Chemistry*
- *Journal of the American Society for Mass Spectrometry*
- *Journal of Chemical Information and Modeling*
- *Frontiers in Inorganic Chemistry*
- *Organic Letters*
- *Journal of Organic Chemistry*
- *European Journal of Organic Chemistry*
- *Organic and Biomolecular Chemistry*
- *Tetrahedron*
- *Journal of Physical Organic Chemistry*
- *Physical Chemistry Chemical Physics*
- *Journal of Physical Chemistry*
- *Journal of Physical Chemistry Letters*
- *Chemical Physics Letters*

2022	Member of the Scientific Advisory Board of the 2nd International Conference on Excited State Aromaticity and Antiaromaticity
2021-2022	Member of the Scientific Committee of the European Young Chemists' Meeting 2022
2021-2022	Co-editor of the *Rosarium Philosophorum on Computational Chemistry*, published by the *Israel Journal of Chemistry*
Since 2020	Member of the Editorial Advisory Board of *ChemistryOpen*
2018	Coauthor of an invited Conference Report on the 2018 ISRIUM Conference for CHIMIA
2018	Coauthor of an invited Conference Report on the 53rd Bürgenstock Conference for CHIMIA
2018-2019	Vice-Chairperson of the Society for Women in Natural Sciences, ETH Zurich
2011-2013	Chairperson of the Organizing Committee, 5th, th and 7th Schulich Graduate Symposium
2009-2010	Member of the Organizing Committee, 3rd and 4th Schulich Graduate Symposium

Teaching Experience – Expanded

As Lecturer at ETH Zurich

Semester	Job	Course
Spring 2021	Lecturer	Organic Chemistry IV: Physical Organic Chemistry
Spring 2020	Lecturer	Organic Chemistry IV: Physical Organic Chemistry
Spring 2019	Lecturer	Organic Chemistry IV: Physical Organic Chemistry
Spring 2018	Lecturer	Organic Chemistry IV: Physical Organic Chemistry

As Teaching Assistant at Technion

Semester	Job	Course	Score *(of 5)*
Winter 2015	Senior Teaching Assistant	Structure Determination Phys. Methods	4.84
Spring 2014	Senior Teaching Assistant	Organic Chemistry 2, Expanded	4.72
Winter 2014	Senior Teaching Assistant	Structure Determination Phys. Methods	4.44
Winter 2014	Senior Teaching Assistant	Organic Chemistry 1, Expanded	4.69
Spring 2013	Senior Teaching Assistant	Organic Chemistry 2, Expanded	4.67
Spring 2013	Senior Teaching Assistant	Structure Determination Phys. Methods	4.64
Winter 2013	Senior Teaching Assistant	Organic Chemistry 1, Expanded	4.58
Spring 2012	Senior Teaching Assistant	Organic Chemistry 2, Expanded	4.80
Spring 2012	Senior Teaching Assistant	Structure Determination Phys. Methods	4.73
Winter 2012	Senior Teaching Assistant	Principles of Chemistry A	4.31
Spring 2011	Senior Teaching Assistant	Organic Chemistry 2, Expanded	4.67
Spring 2010	Teaching Assistant	Organic Chemistry 2, Expanded	4.76
Winter 2010	Senior Teaching Assistant	Structure Determination Phys. Methods	4.94
Winter 2010	Teaching Assistant	Organic Chemistry 1, Expanded	4.67
Spring 2009	Teaching Assistant and Lab Instructor	Principles of Chemistry B	4.27
Winter 2009	Senior Teaching Assistant	Organic Chemistry 1, Expanded	4.83
Winter 2009	Teaching Assistant	Principles of Chemistry A	4.13
Spring 2008	Teaching Assistant and Lab Instructor	Principles of Chemistry B	4.79
Winter 2008	Teaching Assistant and Lab Instructor	Principles of Chemistry A	4.24