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List of Publications and Software

March 2025

Notes: 1) * denotes corresponding author. 2) Titles in red are clickable links.

Peer-Reviewed Publications

48. Y. Davidson, A. Philipp, S. Chakraborty, A. M. Bronstein*, and R. Gershoni-Poranne*
How Local is 'Local'? Deep Learning Reveals Locality of the Induced Magnetic Field of Polycyclic Aromatic Hydrocarbons
Journal of Chemical Physics **2025**, *Accepted*

47. F. Khaleel, S. Chakraborty, and R. Gershoni-Poranne*
Polybenzenoid Hydrocarbons in the S_1 State: Simple Structural Motifs Predict Electronic Properties and (Anti)Aromaticity
Journal of Physical Organic Chemistry **2025**, *Accepted*

46. K. Dey, A. Gorai, K. Mlodzikowska-Pienko, N. Fridman, I. Avigdori, R. Gershoni-Poranne*, and G. de Ruiter*
Manganese-Ketenimine Intermediates as Active Catalysts in the Michael Addition of Unactivated Nitriles to α,β-Unsaturated Ketones
Angewandte Chemie International Edition **2025**, *Accepted Article*.

45. Y. Zhu, Z. Zhou, Z. Wei, A. Tsybizova, R. Gershoni-Poranne*, and M. A. Petrukhina*
Stabilizing Contorted Doubly-Reduced Tetraphenylene with Heavy Alkali Metal Complexation: Crystallographic and Theoretical Evidence
Chemistry – An Asian Journal **2025**, *Early View*.

44. A. Wahab and R. Gershoni-Poranne*
Accelerated Diradical Character Assessment in Large Datasets of Polybenzenoid Hydrocarbons Using xTB Fractional Occupation
Physical Chemistry Chemical Physics **2025**, *Advance Article*.
⇒ **Featured on the *Inside Front Cover***

43. G. I. Warren, K. Mlodzikowska-Pienko, S. Jalife, I. S. Demachkie, J. I. Wu, M. M. Haley, and R. Gershoni-Poranne*
Effects of Benzoheterocyclic Annelation on the s-Indacene Core: a Computational Analysis
Chemical Science **2025**, *16*, 575.
⇒ **Featured on the *Inside Front Cover***

42. S. Garhwal, S. Raje, K. Mlodzikowska-Pienko, T. S. Mohammed, R. Rafaeli, N. Fridman, L. J. W. Shimon, R. Gershoni-Poranne*, and G. de Ruiter*
N_2 Dissociation vs. Reversible 1,2-Methyl Migration in PCNHCP Cobalt(I) Complexes in the Stereoselective Isomerization (E/Z) of Allyl Ethers
JACS Au **2024**, *4*, 4234.
⇒ **Featured as a *Supplementary Front Cover***

41. Y. Zhu, Z. Zhou, Z. Wei, A. Tsybizova, R. Gershoni-Poranne*, and M. A. Petrukhina*
What a Difference an Electron Makes: Structural Response of Saddle-Shaped Tetraphenylene to One and Two Electron Uptake
ChemistryEurope **2024**, *2*, e202400055.
⇒ **Featured on the *Front Cover***
⇒ **Highlighted in *ChemistryViews***

40. S. Chakraborty, E. Mayo Yanes, and R. Gershoni-Poranne*
Hetero-Polycyclic Aromatic Systems: A Data-Driven Investigation of Structure-Property Relationships
Beilstein Journal of Organic Chemistry **2024**, *20*, 1817.

39. A. Wahab and R. Gershoni-Poranne*
COMPAS-3: a dataset of peri-condensed polybenzenoid hydrocarbons
Physical Chemistry Chemical Physics **2024**, *26*, 15344.

38. S. Jalife, A. Tsybizova, R. Gershoni-Poranne*, and J. I. Wu*
Modulating Paratropicity in Heteroarene-Fused Expanded Pentalenes
Organic Letters **2024**, *26*, 1293.

37. E. Mayo Yanes, S. Chakraborty, and R. Gershoni-Poranne*
COMPAS-2: a Dataset of Cata-Condensed Hetero-Polycyclic Aromatic Systems
Scientific Data **2024**, *11*, 97.

36. Z. Yang, R. Nandi, A. Orieshyna, R. Gershoni-Poranne, S. Zhang*, and N. Amdursky*
Light-Triggered Enhancement of Fluorescence Efficiency in Organic Cages
Journal of Physical Chemistry Letters **2023**, *15*, 136.

35. T. Weiss, E. Mayo Yanes, S. Chakraborty, A. M. Bronstein* and R. Gershoni-Poranne*
Guided Diffusion for Inverse Molecular Design
Nature Computational Science **2023**, *3*, 873.
⇒ **Featured on the *Front Cover***
⇒ **Highlighted in *News & Views***

34. M. Pennachio, Z. Wei, R. G. Clevenger, K. V. Kilway, A. Tsybizova, R. Gershoni-Poranne,* and M. A. Petrukhina*
Repercussions of Multi-Electron Uptake by a Twistacene: A Reduction-Induced Double Dehydrogenative Annulation
Organic Chemistry Frontiers **2023**, *10*, 5823.
⇒ **Featured on the *Inside Front Cover***

33. R. Gershoni-Poranne* and A. Tsybizova
A Crowning Achievement: The First Solution-Phase Synthesis of Circumcoronenes
Angewandte Chemie Int. Ed. **2023**, *62*, e202305289.

32. T. Weiss, A. Wahab, A. M. Bronstein and R. Gershoni-Poranne*
Interpretable Deep-Learning Unveils Structure-Property Relationships in Polybenzenoid Hydrocarbons
Journal of Organic Chemistry **2023**, *88*, 9645.
⇒ **Featured on the *Front Cover***

31. M. Pennachio, Z. Zhou, Z. Wei, A. Tsybizova, R. Gershoni-Poranne*, and M. A. Petrukhina*
Interplay of Charge and Aromaticity Upon Chemical Reduction of p-Quinquephenyl with Alkali Metals
Organometallics **2023**, *42*, 2492.

30. S. Fite, A. Wahab, E. Paenurk, Z. Gross and R.Gershoni-Poranne*
Text-Based Representations with Interpretable Machine Learning Reveal Structure-Property Relationships of Polybenzenoid Hydrocarbons
Journal of Physical Organic Chemistry **2022**, *36*, e4458.
⇒ **Invited contribution for the special issue on *Excited State Aromaticity and Antiaromaticity***

29. A. Wahab, L. Pfuderer, E. Paenurk, and R. 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.
⇒ **Featured on the *Front Cover***

28. Z. Zhou, D. T. Egger, C. Hu, M. Pennachio, Z. Wei, R. K. Kawade, Ö. Üngör, R. Gershoni-Poranne,* M. A. Petrukhina*, and I. V. Alabugin*
Localized Antiaromaticity Hot-spot Drives Reductive Dehydrogenative Cyclizations in Bis- and Mono-Helicenes
Journal of the American Chemical Society **2022**, *144*, 12321.
⇒ **Featured on the *Front Cover***

27. E. Paenurk* and R. Gershoni-Poranne*
Simple and Efficient Visualization of Aromaticity: Bond Currents Calculated from NICS Values
Physical Chemistry Chemical Physics **2022**, *24* 8631.
⇒ **Featured on the *Front Cover***

26. R. Thenarukandiyil, E. Paenurk, A. Wong, N. Fridman, A. Karton, R.Carmieli, G. Ménard, R.Gershoni-Poranne,* and G.de Ruiter*
Extensive Redox Non-Innocence in Iron Bipyridine-Diimine Complexes: a Combined Spectroscopic and Computational Study
Inorganic Chemistry **2021**, *60*, 18296.

25. Z. Zhou, Ö. Üngör, Z. Wei, M. Shatruk*, A. Tsybizova, R. Gershoni-Poranne,* and M. A. Petrukhina*
Tuning Magnetic Interactions Between Triphenylene Radicals by Variation of Crystal Packing in Structures with Alkali Metal Counterions
Inorganic Chemistry **2021**, *60*, 14844.

24. G. Markert, E. Paenurk, and R. 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***
⇒ **Denoted as a *Hot Paper***

23. E. Paenurk, S. Feusi, and R. 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***

22. M. A. Hope, T. Nakamura, P. Ahlawat, A. Mishra, M. Cordova, F. Jahanbakhshi, M. Mladenović, R. Runjhun, L. Merten, A. Hinderhofer, B. I. Carlsen, D. J. Kubicki, R. Gershoni-Poranne, T. Schneeberger, L. C. Carbone, Y. Liu, S. M. Zakeeruddin, J. Lewinski, A. Hagfeldt, F. Schreiber, U. Rothlisberger, M. Grätzel*, J. V. Milić*, and L. Emsley*
Nanoscale Phase Segregation in Supramolecular pi-Templating for Hybrid Perovskite Photovoltaics from NMR Crystallography
Journal of the American Chemical Society **2021**, *143*, 1529.

21. T. Schnitzer, E. Paenurk, N. Trapp, R. Gershoni-Poranne, and H. Wennemers*
Peptide–Metal Frameworks with Metal Strings Guided by Dispersion Interactions
Journal of the American Chemical Society **2021**, *143*, 644.

20. A. Wahab, F. Fleckenstein, S. Feusi, and R. 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**
⇒ **Selected as *Editor's Choice* paper**

19. E. Solel, D. Pappo, O. Reany, T. Mejuch, R. Gershoni-Poranne, M. Botoshansky, A. Stanger, and E. Keinan*
Flat corannulene: when a transition state becomes a stable molecule
Chemical Science **2020**, *11*, 13015.

18. S. Eichenberger, M. Hönig, M. J. R. Richter, R. Gershoni-Poranne,* and E. M. Carreira*
Ring-fused cyclobutanes via cycloisomerization of alkylidenecyclopropane acylsilanes
Chemical Science **2020**, *11*, 5294.

17. M. A. Ruiz-Preciado, D. J. Kubicki, A. Hofstetter, L. McGovern, M. H. Futscher, A. Ummadisingu, R. Gershoni-Poranne, S. M. Zakeeruddin, B. Ehrler, L. Emsley*, J. V. Milić*, and M. Grätzel*
Supramolecular Modulation of Hybrid Perovskite Solar Cells via Bifunctional Halogen Bonding Revealed by Two-Dimensional ^{19}F Solid-State NMR Spectroscopy
Journal of the American Chemical Society **2020**, *142*, 1645.

16. 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.

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

14. J. V. Milić, C., N. Hellou, F. Isenrich, R. Gershoni-Poranne, D. Neshchadin, S. Egloff, N. Trapp, L. Ruhlmann, C. Boudon, G. Gescheidt, J. Crassous, and F. Diederich*
Light-Responsive Pyrazine-Based Systems: Probing Aromatic Diarylethene Photocyclization
Journal of Physical Chemistry C **2018**, *122*, 19100.

13. 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.

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

11. S. Künzi, R. Gershoni-Poranne, and P. Chen*
Mechanistic Studies on the Nickel-Catalyzed Cyclopropanation with Lithiomethyltrimethylammonium Triflate
Organometallics **2019**, *38*, 1928.

10. P. Chen* and R. Gershoni-Poranne
Response to "Covalent Bonding and Charge Shift Bonds: Comment on 'The Carbon–Nitrogen Bonds in Ammonium Compounds Are Charge Shift Bonds'"
Chemistry – A European Journal **2017**, *23*, 18325.

9. E. Paenurk, R. Gershoni-Poranne, and P. Chen*
Trends in Metallophilic Bonding in Pd-Zn and Pd-Cu Complexes
Organometallics **2017**, *36*, 4854.

8. R. Gershoni-Poranne and P. Chen*
The C-N Bonds in Ammoniums are Charge Shift Bonds
Chemistry – A European Journal **2017**, *23*, 4659.

7. R. Gershoni-Poranne and A. Stanger*
Magnetic Criteria of Aromaticity
Invited Review Chemical Society Reviews **2015**, *44*, 6597.

6. M. Schaffroth, R. Gershoni-Poranne, A. Stanger*, and U. H. F. Bunz*
Tetraazacenes Containing Four-membered Rings in Different Oxidation States. Are They Aromatic? A Computational Study
Journal of Organic Chemistry **2014**, *79*, 11644.

5. R. Gershoni-Poranne and A. Stanger*
The NICS-XY-Scan: Identification of Local and Global Ring Currents in Multi-Ring Systems
Chemistry – A European Journal **2014**, *20*, 5673.

4. R. Gershoni-Poranne, C. M. Gibson, P. W. Fowler, and A. Stanger*
Concurrence between Current Density, Nucleus-Independent Chemical Shifts, and Aromatic Stabilization Energy: The Case of Isomeric [4]- and [5]Phenylenes
Journal of Organic Chemistry **2013**, *78*, 7544.

3. R. Gershoni-Poranne and A. Stanger*
An MO-Based Identification of Charge-Shift Bonds
ChemPhysChem **2012**, *13*, 2377.

2. M. Standera, R. Haefliger, R. Gershoni-Poranne, A. Stanger, G. Jeschke, J. D. van Beek, and A. D. Schlüter*
Evidence for Fully Conjugated Double-Stranded Cycles
Chemistry – A European Journal **2011**, *17*, 12163.

1. R. Gershoni-Poranne, D. Pappo, E. Solel, and E. Keinan*
Corannulene Ethers Via Ullmann Condensation
Organic Letters **2009**, *11*, 5146.

Preprint / Under Review

2. S. Chakraborty, Itay Almog, and R. Gershoni-Poranne*
   COMPAS-4: a Dataset of $(BN)_1$-Substituted Cata-Condensed Polybenzenoid Hydrocarbons – Data Analysis and Feature Engineering
   Submitted **2025**, *Currently under review at J. Chem. Inf. Model.*

1. B. K. Hillier, D. M. de Clercq, S. D. S. Bortolussi, S. S. Capomolla, M. P. Nielsen, K. Młodzikowska-Pieńko, Renana Gershoni-Poranne, Timothy W. Schmidt*, and Martin D. Peeks*
   Photoexcited and Ground-State Diradical(oid) Character in a Triquino[3]radialene
   Submitted **2025**, *Currently under review at Chem. Sci.*

Book Chapters

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

Software

Notes: All of our software is freely available to download from the *Poranne Group Repository*.

2. BC-Wizard
   Python package implementing the NICS2BC method for calculating bond-currents from NICS values.

1. Predi-XY
   Python package implementing an additivity scheme for rapid generation of NICS-XY-Scans for polycyclic aromatic systems.