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List of Publications and Software

November 2024

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

Peer-Reviewed Publications.....

44. Alexandra Wahab and R. Gershoni-Poranne*
Accelerated Diradical Character Assessment in Large Datasets of Polybenzenoid Hydrocarbons Using xTB Fractional Occupation
Physical Chemistry Chemical Physics **2024**, *accepted*.
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 **2024**, *accepted*.
⇒ **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*.
N₂ Dissociation vs. Reversible 1,2-Methyl Migration in PCNHCP Cobalt(I) Complexes in the Stereoselective Isomerization (E/Z) of Allyl Ethers
JACS Au **2024**, *In Press*.
⇒ **Featured on the 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 Pentalenenes
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.
⇒ **Featured on the 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.
⇒ **Featured on the Cover Feature**
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 ¹⁹F Solid-State NMR Spectroscopy
Journal of the American Chemical Society **2020**, 142, 1645.
16. Z. Zhou, R. K. Kawade, Z. Wei, F. Kuriakose, Ö. Üngör, M. Jo, M. Shatruk, R. Gershoni-Poranne*, M. A. Petrukhina*, and I. V. Alabugin*
Negative charge as a lens for concentrating 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.....

1. 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
Submitted **2024**, currently under review.

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.