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List of Publications

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For further citation information, please see Google Scholar Profile.
Notes: 1) * denotes corresponding author. 2) Titles in red are clickable links.

34. Tomer Weiss, Alexandra Wahab, Alex M. Bronstein and Renana Gershoni-Poranne*
Interpretable Deep-Learning Unveils Structure-Property Relationships in Polybenzenoid Hydrocarbons
ChemRxiv, **2022**, *under review, July 2022*.

33. Shachar Fite, Alexandra Wahab, Eno Paenurk, Zeev Gross and Renana Gershoni-Poranne*
Revealing Structure-Property Relationships in Polybenzenoid Hydrocarbons with Interpretable Machine-Learnings
ChemRxiv, **2022**, *under review, July 2022*.

32. 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**, *accepted*.

31. 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*

30. 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*

29. Ranjeesh Thenarukandiyil, Eno Paenurk, Anthony Wong, Natalia Fridman, Amir Karton, Raanan Carmieli, Gabriel Ménard, Renana Gershoni-Poranne*, and Graham de Ruiter*
Extensive Redox Non-Innocence in Iron Bipyridine-Diimine Complexes: a Combined Spectroscopic and Computational Study
Inorganic Chemistry, **2021**, *60*, 18296.

28. 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.

27. 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.

26. 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*

25. 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*

24. 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 -Templating for Hybrid Perovskite Photovoltaics from NMR Crystallography
Journal of the American Chemical Society, **2021**, *143*, 1529-1538.

23. 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*, 644-648.

22. 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

21. 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*, 13015-13025..
Selected for a *Cover Feature*

20. 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*, 5294-5298.

19. 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, 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*, 1645-1654.

18. 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.

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

16. R. Gershoni-Poranne and P. Chen
The 2018 ISRIUM Conference
Invited Conference Report CHIMIA International Journal for Chemistry **2018**, *72*, 666.

15. 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*, 19100-19109.

14. R. Gershoni-Poranne, A. Kolleth
The 53rd Bürgenstock Conference
Invited Conference Report CHIMIA International Journal for Chemistry **2018**, *72*, 436-439.

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*, 14808-14817.

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

11. S. Künzi, R. Gershoni-Poranne, and P. Chen
Mechanistic Studies on the Nickel-Catalyzed Cyclopropanation with Lithiomethyltrimethylammonium Triflate
Organometallics **2019**, *38*, 1928-1938.

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*, 4854-4863.

8. R. Gershoni-Poranne and P. Chen
The C-N Bonds in Ammoniums are Charge Shift Bonds
Chemistry – A European Journal **2017**, *23*, 4659-4668

7. R. Gershoni-Poranne and A. Stanger
Magnetic Criteria of Aromaticity
Invited Review Chemical Society Reviews **2015**, *44*, 6597-6615.

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*, 11644-11650.

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*, 5673-5688.

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*, 7544-7553.

3. R. Gershoni-Poranne and A. Stanger
An MO-Based Identification of Charge-Shift Bonds
ChemPhysChem **2012**, *13*, 2377-2381.

2. M. Standera, R. Haefliger, R. Gershoni-Poranne, A. Stanger, G. Jeschke, J. D. van Beek, and A. D. Schlüter
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1. R. Gershoni-Poranne, D. Pappo, E. Solel, and E. Keinan
Corannulene Ethers Via Ullmann Condensation
Organic Letters **2009**, *11*, 5146-5149.