

Aromatic rings in porphyrins and their naturally occurring derivatives are among the most important chemical individuals in the world: no aerobic life on this planet can do without the characteristic carbon- and nitrogen-based macrocycles, which carry oxygen in the bloodstream (as a part of hemoglobin) and allow plants to capture sunlight's energy with their chloroplasts. Over the last decades the exceptional electron-transport and energy-harnessing capabilities of the macro- and polycyclic aromatic species have been utilized in cancer therapy, drug delivery, bio-imaging, molecular electronics, solar cells, lighter converters, bio-sensors, quantum computing, photoluminescent materials, photodetectors, and many, many others, making aromaticity one of the most commonly exploited theoretical concepts in chemistry – according to the ISI Web of Science, in 2018 there were about 45 papers published every day that contained the word 'aromatic' (or its antithesis) in title, keywords or abstract. On the other hand, the lack of a rigorous definition and the resulting superfluous diversity (dozens of types and rules of aromaticity) and numerous examples of the discrepancies between different aromaticity criteria proposed in the literature, have become the main reasons for this concept being perceived by some members of the chemical community as an elusive, questionable and suspicious concept. But, if rightly?

In this project we propose a profound paradigmatic change of the concept of (anti) aromaticity, to reveal its true colors and unearth its real predictive power, based on the following scientific hypotheses:

1. Chemical resonance underlying electron delocalization is essentially of information-entropic nature: the key effect of the interference of different resonance forms is that we lose information on the assignment of electrons to particular bonds;
2. One of the most distinguished features of aromatic compounds is their capacity to counterbalance 'destructive' effects of the electron excitations on the ground-state system of π -conjugated bonds by redistribution of the resonance forms in such a way that maximizes the resonance-entropy production or at least minimizes the resonance-entropy loss to preserve as much information contained in their π -systems as possible.

In this context, the core objective of the project is to decipher information contained in the ground-state wavefunctions of selected topologically diversified aromatic molecules and underlying their unique physico-chemical properties, and to progress toward understanding of the first-principle rules that determine evolution of this information in the lowest-lying excited states, under the influence of external magnetic field as well as along chemical reactions. Verification of the project hypotheses requires cross-disciplinary approaches, using knowledge from mathematics, information theory, theoretical and computational chemistry, and materials science, which makes it a truly exciting multidisciplinary challenge. The project will deliver an original method that holds the promise to open new directions in the field of molecular aromaticity as well as tools and research-based knowledge that could support the design and synthesis of novel conjugated materials for artificial photosynthesis and photoinduced electron transfer, molecular photovoltaics, porphyrinoids with resonance-driven optical-mechanistic switches for nanoscience, nanotechnology and biomedicine, and many others. Validation of the proposed maximum resonance-entropy principle for conjugated systems would have potentially far-reaching implications for predictive computational chemistry as well as organic chemistry in general. A tangible result of the research project will be new software, a website dedicated exclusively to the project outcomes, and scientific open-access papers published in reputed journals from the ISI Master Journal List.