

Although the importance of aromaticity as a central concept in chemistry has not diminished since the discovery of benzene, the universal theoretical strategy to quantify it has not been found. It is well-known, that the electron delocalization effect is at the very heart of the aromaticity phenomenon (usually delocalization pertains only to π electrons in unsaturated organic molecules, but nowadays also the σ - and δ -aromatic stabilization effects are considered; they are especially important in the chemistry of transition metals). Electron delocalization determines nearly all distinguishing physicochemical properties of aromatic systems such as stability and reactivity, molecular geometry, spectroscopic properties (UV/VIS, IR and NMR spectra) and magnetic properties. Unfortunately, quantitative evaluation of the aromatic stabilization effects is very problematic since different methodologies of quantifying these properties may sometimes lead to contradictive conclusions. Over the last decade, a great progress has been achieved in the development of quantum-mechanical measures of the electron delocalization. However, their applicability is cut back mainly due to low universality and high computational costs.

In our research group the new aromaticity index has recently been proposed that is based on the so called electron density of delocalized bonds (EDDB). The EDDB method is free of the aforementioned disadvantages and provides both a detailed description of local aromaticity of selected molecular fragment as well as the bird's-eye view on the global aromaticity of nanoscopic-size molecules like fullerenes, graphene petals or carbon nanotubes.

The main goal of the project is the application of the EDDB method to investigate the influence of the electron delocalization effects on structure and reactivity of selected molecules that has not been investigated so far or are the subject of discussion in the literature. The EDDB method will be used to investigate global and local aromatic stabilization effects in polyacenes, oligothiophenes as well as fused σ -boranes, analyze the influence of structural defects on the circuit and spherical aromaticity in fullerenes, and to explain the multifold aromaticity phenomenon in selected metallacycles. The practical purpose of the project is to develop a universal tool that will provide a user-friendly interface for systematic studies of electron delocalization in molecular systems.

The results of the project will contribute to explain the physicochemical properties of molecules of great importance in catalysis, organic synthesis and material science. In particular, the results of the project will support the development of new catalysts for olefin metathesis and the design of new hydrogen storage materials, assist the interpretation of the phosphorescence spectra of oligothiophenes and provide the new insights into mechanisms of organic synthesis of fullerenes from their aromatic precursors. The developed software will enable studies of local and global effects of the electron delocalization of any type in molecular systems that due to their size and structure are the major challenge for currently used tools.