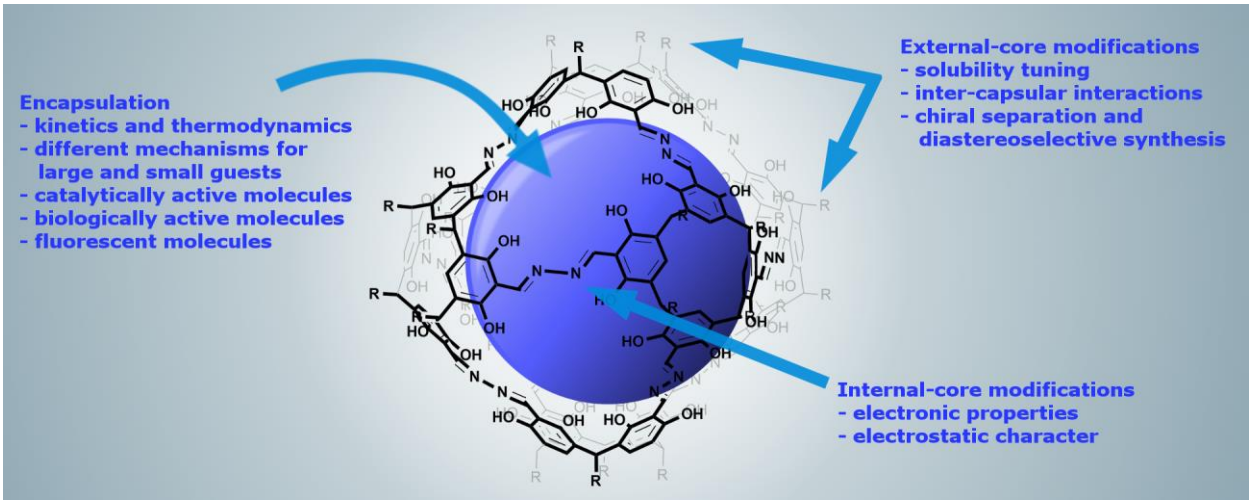
Tuning the properties of organic cubic cages with intrinsic chirality and porosity

1. Research project objectives/Research hypothesis

Molecular containers (capsules or cages) are defined as discrete entities that are able to complex smaller molecules in their interiors and separate/isolate them from the external environment (bulk solvent). They find applications in separation, storage and controlled release of guest molecules. They are also used as reaction nanovessels that provide unusual selectivity and catalytic activity. Recent examples also show their potential in construction of intrinsically porous materials. Recently, we have synthesized a new hexameric molecular container that is distinctively different from all the previously known hexameric capsules - it is formed using covalent but reversible bonds (that makes it stable and controllable), it is chiral (very unique feature among large molecular containers), it has a large cavity surrounded by a rigid skeleton (well-defined complexation space) with molecule-sized portals (possibility of diffusion-controlled encapsulation of small molecules) (Figure below). The objectives of this project are to study the properties of this capsule and to further fine-tune its characteristics towards application-oriented features, i.e., towards development of enzyme-mimicking catalytic systems, intrinsically porous solid materials, drug-delivery systems or materials with modulated fluorescence properties.



2. Research project methodology

The research methodology will involve optimization of the current synthetic procedure (studies on scope and limitation, solvent dependence, catalytic versions and elaboration of conditions for controlled opening); synthesis of new capsules with modified external shells (for solubility tuning or control over inter-capsular interactions for construction of intrinsically porous solids), synthesis of capsules with modified internal core (to modulate electronic character of the interior, potential fluorescence and chirality) and advanced studies on complexation properties (various guests – potential catalysts, drugs, fluorescent dyes; thermodynamics and kinetics of guests' encapsulation and release considering possible different mechanisms for large and small guests, mechanochemical induction of encapsulation).

3. Expected impact of the research project on the development of science

A successful realization of the project will, in the short perspective, provide a set of stable, chiral container molecules with solubilities ranging from water to hydrocarbons (therefore applicable in biological environments), controlled guest entrapment/release (for delivery systems) and tunable intracapsular interactions (for construction of intrinsically porous solids). In the long run, these containers, being themselves a scientific novelty, can find applications in areas that exploit the intrinsic porosity of molecules, especially in areas of catalysis, drug delivery and material science.