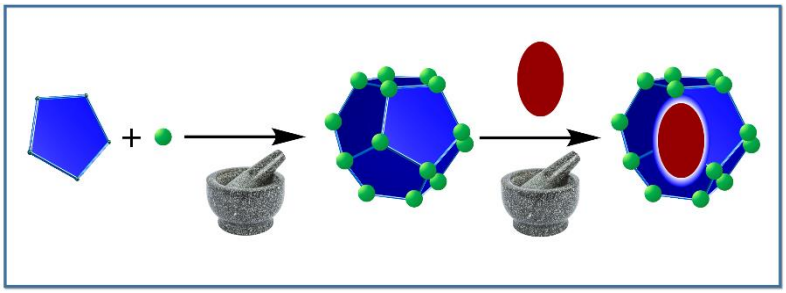
Mechanochemical self-assembly of anion-sealed molecular capsules

Grinding of two solids is historically the first method that was used for carrying out of chemical reactions. This method, dating back to ancient times, have survived in a vestigial form in inorganic chemistry, but it was mostly ignored by 20th century organic chemists. However, recent years have brought an enormous interest in this technique (called mechanochemistry) and in 2019 it was identified by IUPAC as one of the 10 world-changing technologies. The approach based on mechanochemistry offers numerous advantages: it is an eco-friendly method (no waste solvent) that is cheap and easy to execute at various scales (commercial mills of various capacities are available). Moreover, it creates a unique local environment for reactions and processes – the reagents have direct contact which causes high local concentration and they are subject to friction forced. Numerous examples demonstrate that under such conditions many of the reactions proceed faster and even products that are different than in the solution may be favored.

In this project we suggest ***mechanochemistry*** to: (a) ***induce the formation of molecular capsules*** and (b) ***enforce the complexation of guests*** inside the capsules. Despite the simplicity and numerous advantages, the applications of mechanochemistry for such purposes remain only vaguely known. We hypothesize that mechanochemistry will enable the formation of species and their complexes that are hard or even impossible to obtain in the solution. Molecular capsules, that are the ultimate target molecules of this project can find applications as nanovessels for storage, separation, in drug delivery or as enzyme-mimics in catalysis.



Our initial results show that unique novel capsules made of biologically–compatible polyphenol macrocycles and chlorides can be formed by mechanochemistry. Therefore, we expect that the execution of this project will lead to new capsules and their complexes with various guest molecules, which may find applications in biological systems or in catalysis. The research in this field will also increase the general understanding of the mechanisms of mechanochemical processes that leads to increasing of the use of this eco-friendly methodology in supramolecular chemistry.