Porous MOFs and molecular capsules for gas absorption based on anthracene derivatives.

S. Vasylevskyi[1], K. M. Fromm[1]*

[1]University of Fribourg

The synthesis and study of new functional materials for the adsorption of potentially valuable energetic gases is an extremely demanding area in modern chemistry, since we have global warming issues causing climate change and natural disasters as a result. Therefore, reduction of the amount of CO_2 and CH_4 in the atmosphere is crucial for the "green" future of our globe.[1-2] Secondly, the high partial pressure of hydrogen can be decreased upon adsorption processes by porous materials which gives the possibility of sorption, storage and transportation of molecular hydrogen.[3] Then the absorbed hydrogen can be easily used as a fuel for industry and for cars due to its green product upon combustion with oxygen.[4] Thus, the synthesis of new materials for such purposes, especially metal organic frameworks (MOFs) is one of the key directions.

At this SCS meeting we will present new MOFs and coordination compounds of Ni(II), Cu(II) and Zn(II) which have been synthesized with anthracene derived ligands. Their crystal structure (Fig. 1a-b) was determined by single crystal *x-ray* diffraction. The complexes show different types of voids: open infinite 1-D channels with diameters ranging from 8 to 20 Å, as well as 0-D capsules. Estimating the porosity by calculation with the crystallographic program PLATON, the complexes show 37-50% of porosity. The determination of the sorption capacity by BET for CO_2, CH_4 and H_2 for the Ni-MOF and the capsule compounds of Cu(II) and Zn(II) will complete the study.

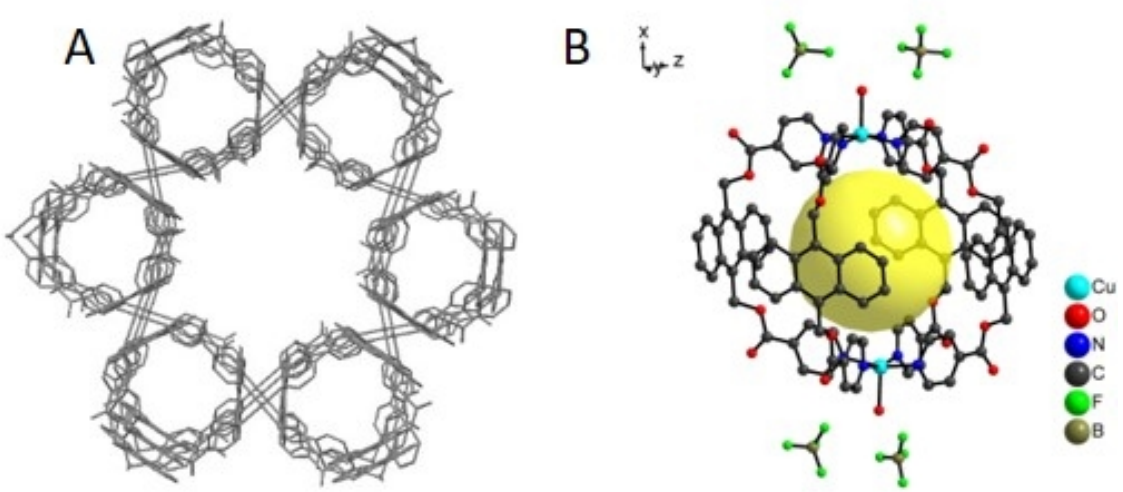

Fig 1. A) Hexagonal structure of Ni-MOF $\{[Ni(L)_4Cl_2]\}_n$ with pore size 8×8 Å and 20×20 Å. B) Structure of Cu-capsule $\{[Cu_2(L)_4(H_2O)_2](BF_4)_4\}_n$.

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