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SUPSI

Hybrid metal-organic nanocages: structures and properties by a combination of XRay and QM studies

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In this contribution, some of the features of poly-[n]-catenanes composed of interlocked $M_{12}L_8$ icosahedral nanometric cages are presented as obtained by a combination of X-ray diffraction experiments and Quantum Mechanical (QM) calculations [1-3]. The TPB (exotridentate trispyridyl benzene) ligand and ZnX_2 (with X=Cl, Br, I), with appropriate templating solvent molecules, form metal−organic interlocked nanocages microcrystalline materials (see Figure 1). X-ray data allowed to solve the structure and to detect guest molecules exchange together with crystal to crystal phase transitions. The processes of crystallization, absorption/release of guests and crystal to crystal transitions are driven by intramolecular and intermolecular interactions. QM calculations specific for the solid phases [4-6] were used to rationalize the observed features permitting to highlight the underlying key factors by a simple hierarchical mechanism of "closed-open" dynamic channels. The capability of specific molecular absorption/release together with the labile nature of the Zn−N coordination bonds allow for the recyclability of TPB ligand and make these materials potential good candidates in green chemistry processes and in molecular sensing and in drug delivery (for example paracetamol) applications (see Figure 2).

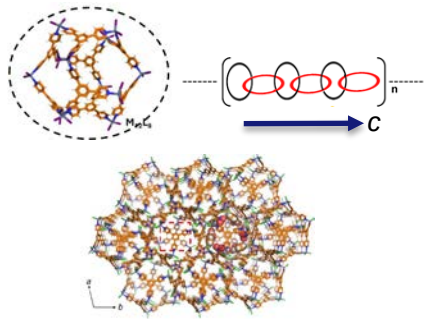

Fig.1 Nanocage, polycatenane, structure.

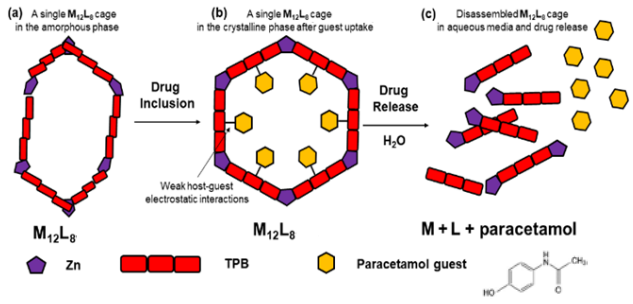

Figure 2 Sketch of inclusion/release of paracetamol molecules.

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