Molecular Adsorbing Host•Guest (MAHG) crystals

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Recently, porous organic crystals (POC) based on macrocycles have shown exceptional sorption and separation properties.[1] Yet, the impact of guest presence inside a macrocycle prior to crystallization and adsorption had not been studied. We will present results about the inclusion of trimethoxybenzyl-azaphosphatrane in the macrocycle cucurbit[8]uril (CB[8]) affording *molecular* adsorbing host•guest crystals (**MAHG**, Figure 1).[2]

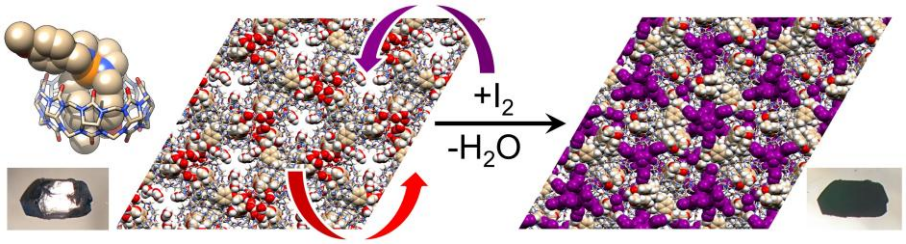

Figure 1. Host•guest complex with CB[8], packing showing 1D channels and iodine adsorption.

Not only the guest could tune the porous space of CB[8] crystals, but also unactivated **MAHG** crystals could adsorb iodine spontaneously and selectively at room temperature and atmospheric pressure. The absence of (i) heat for material synthesis, (ii) moisture sensitivity, and (iii) energy-intensive steps for pore activation are attractive attributes to produce energy-efficient porous materials. ^{1}H NMR and DOSY were instrumental for monitoring the H_2O/I_2 exchange and iodine-doped crystals showed markedly different second harmonic generation. Recent results will also be presented highlighting a growing diversity of what could be a new family of porous materials.

References

1. Zhu, H.; Chen, L.; Sun, B.; Wang, M.; Li, H.; Stoddart, J. F.; Huang, F. *Nat. Rev. Chem.* **2023**, *7*, 768-782.
2. Yang, X.; Li, C.; Giorgi, M.; Siri, D.; Bugaut, X.; Chatelet, B.; Gigmes, D.; Yemloul, M.; Hornebecq, V.; Kermagoret, A.; Brasselet, S.; Martinez, A.; Bardelang, D. *Angew. Chem. Int. Ed.* **2022**, *61*, e202214039.