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A bi-porous metal–organic framework with tuneable sorption performance facilitated by intrinsic flexibility

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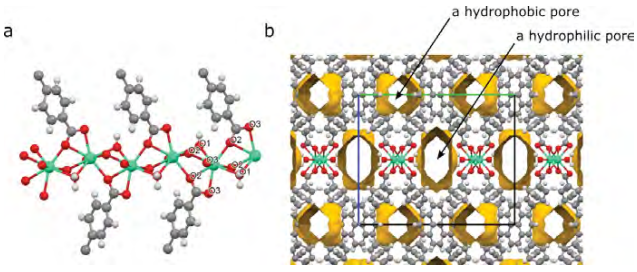
Efficient CO_2/CH_4 separation has constantly been a challenge for natural gas processing, and in general, modern chemical industry.[1] While classical separation techniques including cryogenic distillation or low-temperature chemical absorption are widely in use, they are energetically costly, and present a considerable environmental issue.[2] Porous materials, constantly developed as alternative solutions to these techniques, are showing a great promise.[3] The purpose, however, is not only to design a material with maximum selectivity and working capacity, but also to rationally control and tune its performance. Herein we present the synthesis of a novel MOF based on Ca(II) and a tetracarboxylate ligand $TBAPy^{4-}$ endowed with two chemically distinct types of pores: the hydrophobic and the hydrophilic one. Owing to judicious choice of conditions access is gained to two stages of activation, at which the material shows strikingly different gas sorption performances. The material's intrinsic flexibility helps it to adsorb a higher amount of gas molecules than is allowed by its unexpanded state. The observed preference of adsorbing CO_2 over CH_4 was further studied in fixed-bed breakthrough experiments imitating the real process in an industrial-scale installation. The difference of sorption behaviour on the material was supported by molecular simulations.



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