

Oral Contributions

[MS38-03] Assembling pore networks in organic cage structures using molecular recognition Samantha Y. Chong,

Tom Hasell, Michael E. Briggs, Kim E. Jelfs, Marc A. Little, Marc Schmidtman & Andrew I. Cooper,

Department of Chemistry and Centre for Materials Discovery, University of Liverpool, Crown Street, Liverpool L69 7ZD, UK.

E-mail: s.chong@liv.ac.uk

Interest in the development of microporous materials has been driven by possible applications in areas such as catalysis, gas storage and separation [1-4]. A class of purely organic molecular cage materials has emerged [5-7] that can exhibit significant porosity arising from the internal void of the cage molecules as well as extrinsic porosity from packing in the crystal structure [8]. Our work has focused on covalent imine-linked cages [5,8,9], which exhibit diverse crystal chemistry demonstrated by the existence of polymorphs [10], cocrystals [9,11] and solid solutions [12]. The arrangement of cage modules in the crystal structure has a direct effect on the observed gas adsorption properties of these materials, with the connectivity of the voids critical in determining whether a significant volume is accessible to guests [5,10]. Having a significant degree of control over the crystal packing and thus the pore topology can enable tuning of properties such as surface area. By exploiting molecular recognition by the cage modules, we have developed broad strategies which allow their directed assembly to transform the void networks. We have previously reported the predictable assembly of cage cocrystals using chiral recognition between cage modules [9]. Here we highlight how this approach can be used to modify the pore network for a specific cage, thereby improving gas adsorption properties of the material [11]. We will also demonstrate how guest response can be used to transform cage crystal structures containing isolated voids in the

guest-free state to open structures with connected channels on loading. Finally, for three chemically distinct cages, we examine how formation of a desired void network topology can be promoted by hosting a specific solvent guest in preferred sites which maximise weak host-guest interactions. Subsequent guest removal can result in stable polymorphs, with improved sorption properties; for one cage polymorph, the Brunauer-Emmett-Teller surface area (SABET) was doubled with respect to the originally observed polymorph obtained from synthetic solvent conditions.

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Keywords: microporous materials; cage molecules; molecular crystals