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Hydrogen Bonding in Inclusion Chemistry and Porous Materials

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Hydrogen bonding played an important role in the development of crystal engineering and cocrystal formation, and continues to do so. Our take on hydrogen bonding will focus on its consequences on the functional properties of a number of materials based on how hydrogen bonding directionality effects porosity design and inclusion chemistry. The design of molecular porous materials has focused on the production of intrinsic porosity within a number of interesting materials where the intrinsic voids are defined by capsules (tetrahedra in our examples) and macrocycles (2X2 metallocycles in our examples). The crystal engineering of the macrocycle packing efficiencies can result in the intrinsic voids spaces being connected into pore networks allowing for diffusion of guest species such as gases. We will show how the hydrogen bonding of these intrinsically porous molecules can result in an increased porosity through the creation of extrinsic void space.[1] The inclusion chemistry we have investigated has looked at gas and vapour sorption where we have determined the guest:framework interaction of a number of porous materials. This includes the inclusion chemistry of a number of persistent organic radicals where the hydrogen bonding and Pi-Pi stacking interactions with the flexible host material results in paramagnetic materials whereas the pure radical materials tend towards being diamagnetic.[2] We will also describe our crystallographic insights into gas:framework interactions, especially that of the hydrogen bonding of Carbon Dioxide.[3]

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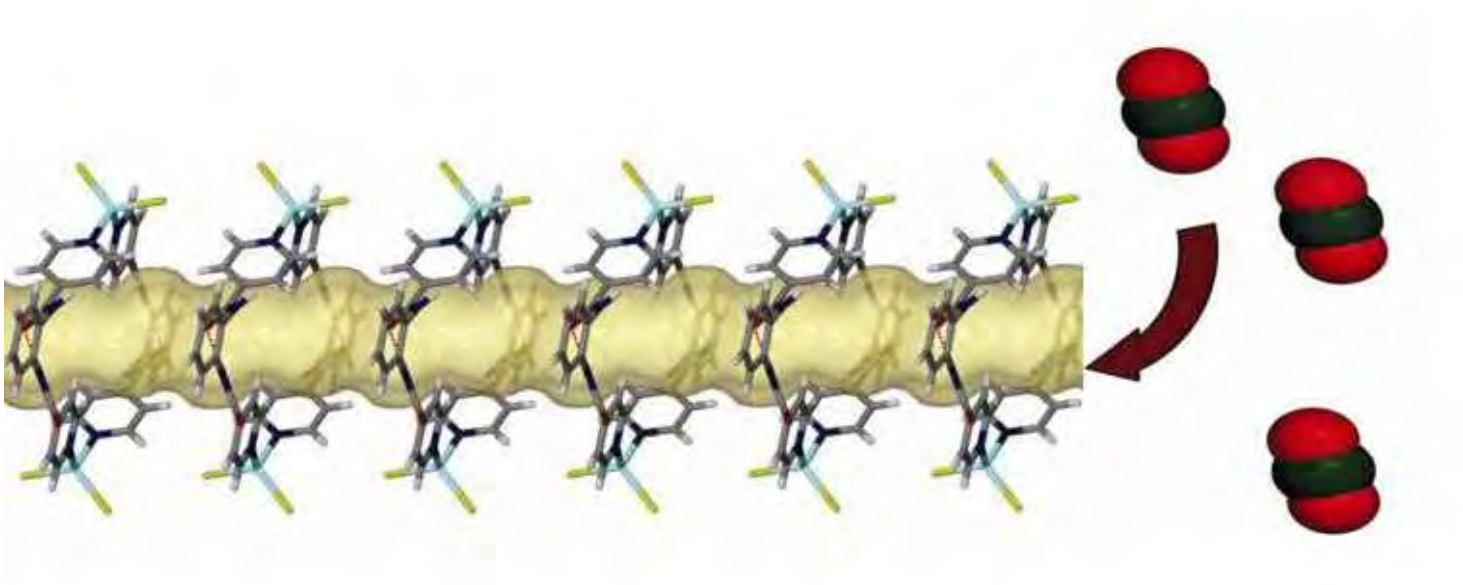

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