

[1] Neutze et al., *Nature* **2000**, *406*, 752-757. [2] D.K. Saldin et al., *J. Phys.: Condens. Matter* **2009**, *21*, 134014. [3] D.K. Saldin et al., *Phys. Rev. B* **2010** *81*, 174105. [4] D.K. Saldin et al. *Phys. Rev. Lett.* **2011**, *106*, 115501. [5] e.g. M. Schmidt et al., In: *Methods in Molecular Biology*, **2005**, Vol. 305, *Protein-Ligand Interactions: Methods and Applications* (G.U. Nienhaus ed.), Humana Press, Totowa, NJ, p. 115 ff.

Keywords: biomacromolecules, X-ray free electron laser

MS.37.5

Acta Cryst. (2011) A67, C93

Imaging biological molecules using X-FELs

Thomas R.M. Barends,^{a,b} the CFEL/ASG Imaging Collaboration^{a,f}, R. Bruce Doake,^k Petra M. L. Fromme,^k John H. Spence,^k Lothar Strüder,ⁿ Joachim Ullrich,^{b,c} Henry N. Chapman,^b Ilme Schlichting,^{a,b} ^aMPI for Medical Research, Heidelberg (Germany). ^bMax Planck Advanced Study Group, Center for Free Electron Laser Science (CFEL), Hamburg, (Germany). ^cMax-Planck-Institut für Kernphysik, Heidelberg (Germany). ^dPNSensor GmbH, München (Germany). ^eCenter for Free-Electron Laser Science, Hamburg (Germany). ^fLaboratory of Molecular Biophysics, Department of Cell and Molecular Biology, Uppsala University, Uppsala, (Sweden). ^gPhoton Science, DESY, Hamburg (Germany). ^hStanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, ⁱLCLS, SLAC National Accelerator Laboratory, Menlo Park, ^jUppsala University, Uppsala (Sweden). ^kDepartment of Physics, Arizona State University, Tempe (USA). ^lDepartment of Physics, Cornell University, Ithaca. ^mDepartment of Chemistry and Biochemistry, Arizona State University, Tempe (USA). ⁿMax-Planck-Institut Halbleiterlabor, München, (Germany). ^oAdvanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, (USA). ^pDepartment of Chemistry, Biochemistry and Biophysics, University of Gothenburg, Gothenburg. ^qUniversity of Hamburg, Hamburg. ^rMax-Planck-Institut für extraterrestrische Physik, Garching. E-mail: Thomas.Barends@mpimf-heidelberg.mpg.de

Tremendously boosted by ever improving synchrotron X-ray sources, X-ray diffraction has been a central tool in structural biology. X-ray free-electron lasers (FELs) provide up to 9 orders of magnitude brighter and much shorter X-ray pulses that may yield diffraction patterns of biological samples before significant radiation damage has occurred (“diffraction before destruction”) [1]. We present results from diffraction experiments with biological samples, both crystalline [2] and single-particle, performed using FEL sources. Analysis of the data shows the potential of FELs for structural biology

[1] R. Neutze, R. Wouts, D. van der Spoel, E. Weckert, J. Hajdu, *Nature* **2011**, *406*, 752-757. [2] H.N. Chapman, P. Fromme, A. Barty, et al. *Nature* **2011**, *470*, 73-77.

Keywords: free electron lasers, nanocrystals, protein crystallography

MS.38.1

Acta Cryst. (2011) A67, C93

Flexible pyrene-derived frameworks for sensing and separation

Darren Bradshaw, Kyriakos C. Stylianou, Romain Heck, John Bacsá, Sam Chong, Jeremy Rabone, Yaroslav Z. Khimyak, Matthew J. Rosseinsky, *Department of Chemistry, University of Liverpool (UK)*. E-mail: deg5y@liverpool.ac.uk

Open frameworks prepared using the well established principles of coordination chemistry are significantly more flexible than their wholly oxide counterparts, leading to novel guest-responsive adsorption behaviors. [1] Such framework flexibility can be pre-determined through the use of deliberately flexible ligands such as dipeptides [2], or can arise from seemingly quite rigid organic linking groups. [3]

The tetracarboxylate ligand 1,3,6,8-tetrakis(*p*-benzoic acid)pyrene (TBAPy) is based on a rigid planar pyrene core, but has sufficient rotational freedom about the benzoate substituents to permit framework dynamics upon metal-binding. This dynamic behavior has been studied using a combined approach of diffraction, solid-state NMR and molecular dynamics simulations.

In this contribution I will present two materials prepared from d¹⁰ metal ions where the structural changes resulting from these benzoate rotations influence the physical properties of the material. Firstly, [In₂(OH)₂(TBAPy)] is a microporous 3-dimensional framework displaying linker-centered emission with a ms lifetime. [4] The emission response is highly dependent on the chemical nature and loading level of guest molecules, and in particular how these affect the framework structure through induced structural changes or specific framework-guest interactions.

Reaction of TBAPy with Zn(II) yields a layered framework of composition [Zn₂(TBAPy)(H₂O)₂] which is linked via the common paddlewheel motif. Large structural changes occur on desolvation, which are consistent with benzoate rotations as evidenced by NMR. Further investigation of the desolvated structure using molecular dynamics simulation reveals a novel rearrangement of the paddlewheel building units transforming the structure into a 3-dimensional porous network that displays modest selectivity for xylene isomers.

[1] S. Horike, S. Shimomura, S. Kitagawa *Nature Chem.* **2009**, *1*, 695-704. [2] J. Rabone et al *Science* **2010**, *329*, 1053-1057. [3] C. Serre et al *Science* **2007**, *315*, 1828-1831. [4] K. Stylianou et al *J. Am. Chem. Soc.* **2010**, *132*, 4119-4130

Keywords: frameworks, flexibility, rearrangement

MS.38.2

Acta Cryst. (2011) A67, C93-C94

Unusual porous functions of stimuli responsive porous coordination polymers

Ryotaro Matsuda,^{a,b} Hiroshi Sato,^{a,b} Joobeom Seo,^{a,b} Susumu Kitagawa,^{a,b,c} ^aExploratory Research for Advanced Technology (ERATO), (Japan) Science and Technology Agency (JST), Kyoto, (Japan). ^bInstitute for Integrated Cell-Material Sciences, Kyoto University, Kyoto, (Japan). ^cDepartment of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Kyoto, (Japan). E-mail: ryotaro.matsuda@kip.jst.go.jp

The discovery of a new nanoporous compound that has unique porous properties is scientifically and technologically topical. In particular, the creation of a porous compound that possesses a switchable pore surface and channel structure is currently a major challenge in material science. This has not yet been realized with currently available materials. The recent advent of porous coordination polymers (PCPs) or metal-organic frameworks (MOFs) as new functional crystalline microporous compounds, has attracted the attention of scientists because of the great practicality of regular nano-sized spaces prepared by simply mixing their organic and inorganic molecular components which result in their finding unusual porous functions such as in storage, catalysis and highly enantio-, size- and shape-selective adsorption. [1]

Here we report new flexible PCPs that show large structural transformation in response to the adsorption of specific guest molecules,