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Metal-Organic Materials: Strategies toward Functional Porous Materials. Mohamed Eddaoudi. Department of Chemistry, The University of South Florida, 4202 E. Fowler Avenue, CHE205, Tampa, Florida, 33620, USA.

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The quest for functional materials targeted for specific applications is ever increasing as societal needs and demands mount with advancing technology. One class of inorganic-organic hybrid materials, metal-organic materials (MOMs), has burgeoned in recent years due, in part, to effective design strategies (i.e. reticular chemistry) for their synthesis and their inherent [and readily interchangeable] hybrid, highly functional character. The molecular building block (MBB) approach introduces the ability to generate rigid and directional building blocks, mostly in situ, for the construction of MOMs having specific underlying networks and/or targeted functions/properties. Here we will discuss three basic strategies based on the MBB approach. Three classes of MBBs can be targeted and utilized in the assembly of functional MOMs: 1) single-metal-ion-based MBBs, which promote the rational construction, by forcing rigidity and directionality through control of the metal coordination sphere and judicious selection of suitable hetero-functional (N-, O- coordination) organic ligands, of porous MOMs with extra-large cavities, including zeolitelike metal-organic frameworks (ZMOFs);1 2) multi-nuclear metal cluster-based MBBs, where, for example, simple metal-carboxylate clusters possess multiple metal-oxygen coordination bonds that result in the generation of rigid nodes with fixed geometry that, when combined with organic ligands of specific geometry, lead to the construction of desired MOMs (e.g. soc-MOFs);² and 3) supermolecular building blocks (SBBs), which involve enhanced built-in directional and structural information (e.g. high degree of symmetry and connectivity) compared to simple MBBs and allow the construction of high-connectivity nets (e.g. rht-MOFs).3 The MBB approach and associated strategies, as well as physical properties of some corresponding MOMs (i.e. porosity, hydrogen sorption, catalysis, inclusion and sensing) will be discussed.



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FA4-MS04-O2

Interpreting Competition Experiments in Host-Guest Chemistry. Luigi R. Nassimbeni. Department of Chemistry, University of Cape Town, South Africa. E-mail: luigi.nassimbeni@uct.ac.za

In order to study the various parameters which determine the affinity between a host and a guest compound in the solid state, we have carried out a series of guest-competition experiments. We have thus exposed a given host to a series of liquid guest mixtures of known composition, varying the mole fractions systematically from 0 to 1. When considering a host H and two guests A and B, with the mole fraction of A, X_A in the liquid, we then determine the mole fraction of this guest in the ensuing crystals, Z_A . A selectivity curve of Z_A vs X_A can then be drawn and a selectivity coefficient $K_{A:B} = Z_A / Z_B * X_B / X_A$ may be calculated at all points along this curve. The value of $K_{A:B}$ is a function of the relative affinities of the host H for the guests A and B.

For a given temperature of crystallization, the questions that arise are:

(i) what are the structures of the solids along the selectivity curve?

(ii) is the selectivity constant dependent on the electronic properties of the guest molecule?

(iii) what is the importance of shape and size of the guest molecule with respect to the packing of the host-guest compound?

Various examples of host-guest selectivity will be presented in order to answer these questions.

Keywords: molecular recognition; competition experiments; selectivity

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Designer Porphyrin Assemblies. Israel Goldberg^a, Sophia Lipstman^a, Sankar Muniappan^a. ^aSchool of Chemistry, Sackler Faculty of Exact Sciences, Tel Aviv University, Israel.

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This presentation addresses the scientific challenge of predictably self-organizing porphyrin molecules into materials with complex topologies, with an emphasis on rational construction of molecular networks and systems exhibiting supramolecular chirality. In order to achieve these goals, the porphyrin scaffold is deliberately functionalised with different molecular recognition groups prone to engage in robust supramolecular synthons. This allows to reasonably control the self-assembly process and to alter systematically the composition and topology of the supramolecular arrays that form. The crystal-engineering approach represents an attractive "bottom-up" strategy to tailoring ordered lattice materials and network architectures