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Towards Anion Recognition and Separation in Metal-Organic Frameworks. Radu Custelcean¹, Maryna G. Gorbunova¹, Peter V. Bonnesen¹, Benjamin P. Hay², Bruce A. Moyer¹, ¹Chemical Sciences Div., Oak Ridge National Laboratory, Oak Ridge, TN 37831, ²Chemical Sciences Div., Pacific Northwest National Laboratory, Richland, WA 99352.

A new approach to the recognition and separation of anions in the solid state will be presented, which employs metal-organic frameworks (MOFs) as scaffolds for the attachment of anion binding sites. This chemistry builds on recent developments in supramolecular chemistry of anions, and coordination polymers. Hydrogen bonding groups such as -OH, COOH, or urea have been incorporated into MOFs via organic synthesis of building blocks containing traditional pyridine or PhCN metal coordinating groups. The design of these ligands was aided by molecular modeling using the HostDesigner software recently developed at PNNL. The MOFs resulting from the self-assembly of the organic ligands with transition metal salts have been analyzed by single crystal X-ray diffraction to assess their anion binding abilities. A particular challenge associated with the design of these materials is to circumvent hydrogen bonding among the anion binding sites, or their coordination to the transition metal nodes. Our crystal engineering efforts along this direction will be highlighted.