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Visualizing Pore Packing and Topology in MOFs

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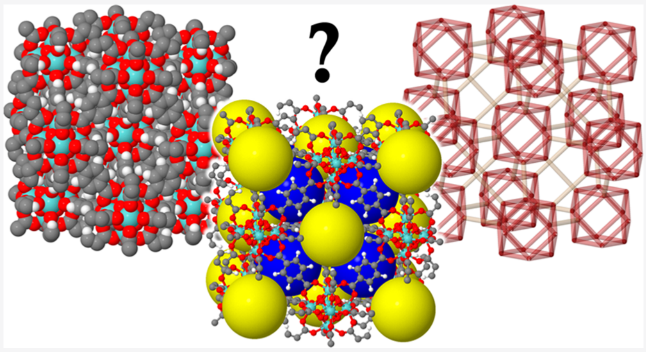
ABSTRACT: Metal organic frameworks (MOFs) can have open pore structures with high surface areas and applications in hydrogen storage, carbon dioxide capture, water harvesting from air, chemical separations, and catalysis. The chemical structure of these crystalline solids can initially appear daunting. Simplification by considering the arrangement of the pores and by identifying the links and vertices as well as switching between multiple representations can make visualization of these structures accessible.



KEYWORDS: *Audience: First-Year Undergraduate/General, Domain: Interdisciplinary, Pedagogy: Analogies/Transfer, Topic: Materials Science, Solid State Chemistry*

Reticular chemistry is the linking of molecular building blocks by strong bonds to make crystalline extended structures.[1] Metal organic frameworks, or MOFs, are products of this chemistry and have become interesting for their open pore structures with high surface areas and applications in hydrogen storage, carbon dioxide capture, water harvesting from air, chemical separations, and catalysis.[2−7]

Publications about MOFs in this journal have primarily concerned synthesis and characterization.[8−19] One report was a study of the impact of including material about MOFs as an introduction to authentic research.[20] Another included model building of MOFs using interlocking disks sold as toys to introduce the topology of primary and secondary building units,[21] discussed further below.

Currently, over 100,000 MOFs have been reported with nearly 500,000 predicted.[22−25] To an incoming student interested in MOFs the task of deciphering MOF structures is daunting not just for their sheer number but also because their structures can initially appear complicated. However, many MOF structures can be reduced in a systematic fashion into simpler basic forms, which in themselves are familiar to students. The goal of this paper is to identify and illustrate the key connections that students can make with their prior knowledge of such simpler forms to enhance comprehension of MOF structures.

■ SPHERE PACKING

One way to simplify framework structures is to view the sphere packing arrangement of their pores. Visualizing where the atoms are not located is a complementary skill to visualizing where the atoms are located. This simplification makes use of known crystal structures, and cubic examples will be used here.

Packing of spheres has been a useful way to describe metallic structures at the atomic level. Most introductory courses mention the primitive cubic, body-centered cubic, and face-centered cubic structures exhibited by more than 30 elements. Filling the spaces between the anions with cations leads to ionic structures. The NaCl, ZnS, and CaF_2 structures are prototypical[26] and were correctly described by W. H. and W. L. Bragg in 1915.[27] (The Braggs originally listed CsCl as isomorphous with NaCl, and it was not until 1921 that the correct structure was suggested.[28])

Figures 1−8 show a cubic unit cell for each of these classic structures in the upper left. The additional panels contain a cubic unit cell of pores in a MOF along with more than a unit cell of the actual MOF structure. Each of these structures can be interactively viewed online. See the Multiple Representations section below.

Figure 1 shows the primitive cubic structure of polonium in comparison with the primitive cubic arrangement of pores in the IRMOF[29] series of isoreticular structures. Figure 2 shows the CsCl structure where the atom in the center of the unit cell is different than the atom on the corners of the unit cell.

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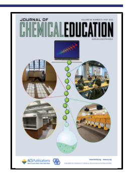

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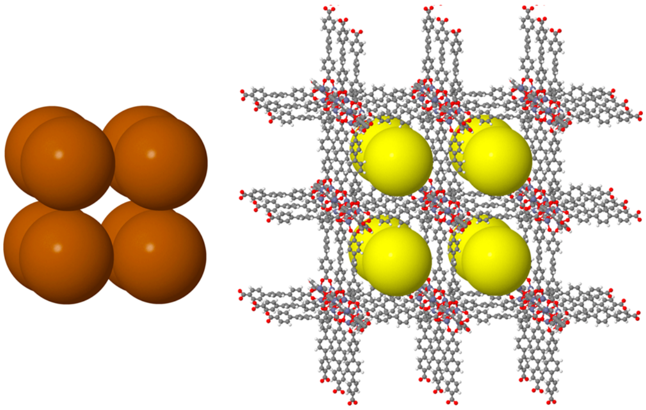

Figure 1. Left: Primitive cubic polonium. Right: IRMOF-16 with 15 Å spheres in the spaces. (The pores are not strictly crystallographically equivalent unless the link ring orientations are disordered.)

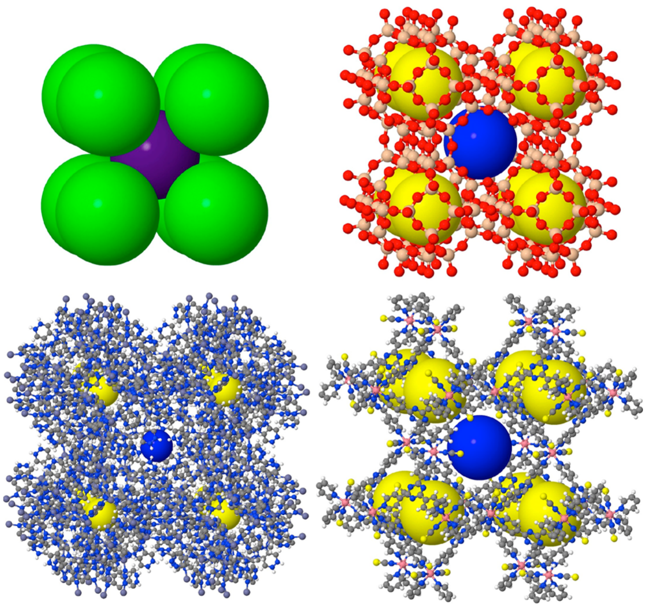

Figure 2. Top left: CsCl salt. Top right: Zeolite A with 7 Å spheres in two types of spaces. Bottom left: ZIF-20 with 6 Å spheres in two types of spaces. Bottom right: MOF-TPT with 10 Å spheres in two types of spaces.

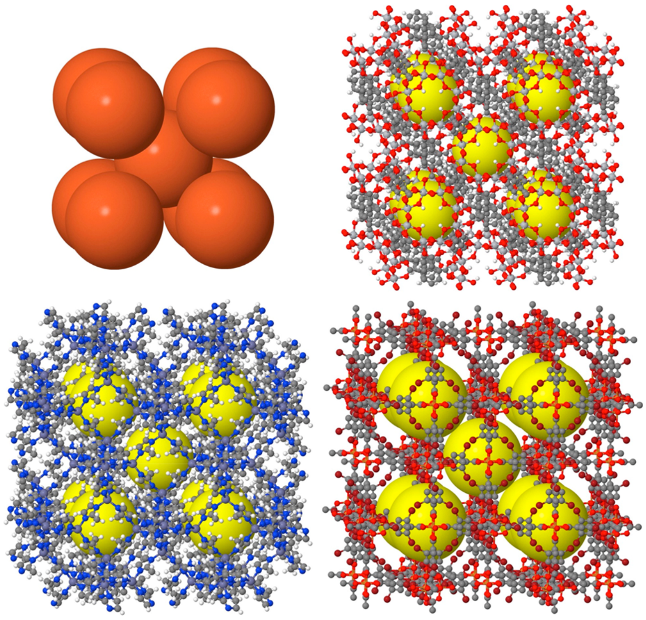

Figure 3. Top left: Body-centered cubic Fe. Top right: MIL-125 with 10 Å spheres in the spaces. Bottom left: ZIF-8 with 10 Å spheres in the spaces. Bottom right: MOF-101 with 14 Å spheres in the spaces.

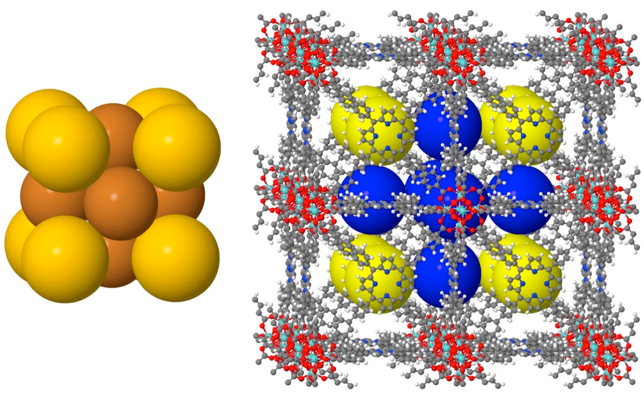

Figure 4. Left: Cu_3Au alloy. Right: NU-1102 with 12 Å spheres in two types of spaces.

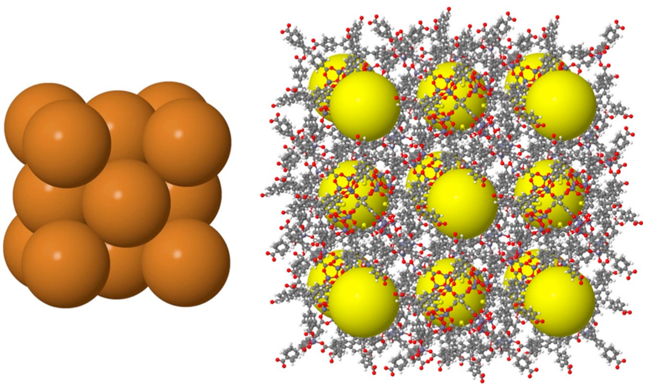

Figure 5. Left: Face-centered cubic Cu. Right: UMCM-3 with 16 Å spheres in the spaces.

Zeolite A,[30] ZIF-20,[31] and MOF-TPT[32] are framework structures with two kinds of pores: one located on the corners of the cubic unit cell and one located in the center. In the CsCl structure, either atom could be viewed as the corner since the structure comprises two interpenetrating primitive cubic arrangements such that one set sits in the cubic holes of the other set. Figure 3 shows the body-centered cubic structure exhibited by Li, Na, K, Rb, Cs, Ba, Ra, V, Nb, Cr, Mo, W, Mn, and Fe, where the atom in the center of the unit cell is the same as the atom on the corners of the unit cell. MIL-125,[33] ZIF-8,[34] and MOF-101[35] are framework structures with a body-centered cubic arrangement of pores. Figure 4 shows the Cu_3Au structure, also exhibited by Pt_3Ag, Fe_3Ga, Fe_3Sn, Cr_3Nb, Bi_3Hg, Ce_3In, Ir_3Ta, Os_3Hf, Yb_3Mg, and Nb_3Si. In the Cu_3Au structure, Au atoms are located on the corners of the cubic unit cell and Cu atoms are located on the faces. NU-1102[36] is a MOF example with two types of pores: one located on the corners of the cubic unit cell and one located on the faces. Figure 5 shows the face-centered cubic structure exhibited by Ca, Sr, Rh, Ir, Ni, Pd, Pt, Cu, Ag, Au, Al, Pb, Yb, Ac, and Th and solid Ne, Ar, Kr, Xe, and Rn. The atom located on each of the faces is the same as the atom on the corner of the unit cell. UMCM-3[37] is a MOF example of a

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framework with identical pores on the corners and faces of the cubic unit cell.

The NaCl structure shown in Figure 6 has a face-centered cubic arrangement of one atom with the other atom located on

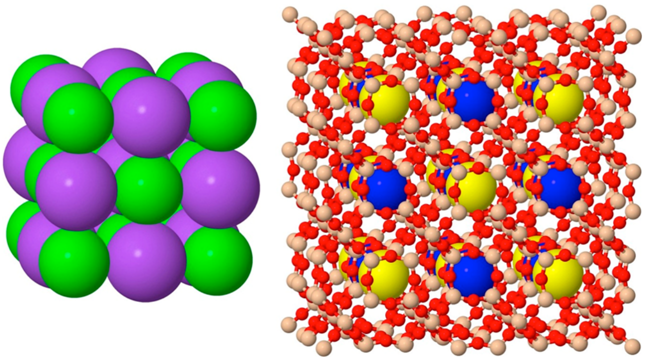

Figure 6. Left: NaCl. Right: AlPO-16 with 4 Å spheres in the spaces.

the 12 edges of the cubic unit cell. ALPO-16[30] is an example of a framework structure with two types of pores; one set is located on the corners and faces while the other set is located on the cell edges. In the NaCl structure either atom could be viewed as the corner since the structure comprises two interpenetrating face-centered cubic arrangements such that one set sits in the octahedral holes of the other set. The CaF_2 (fluorite) structure in Figure 7 is a face-centered cubic

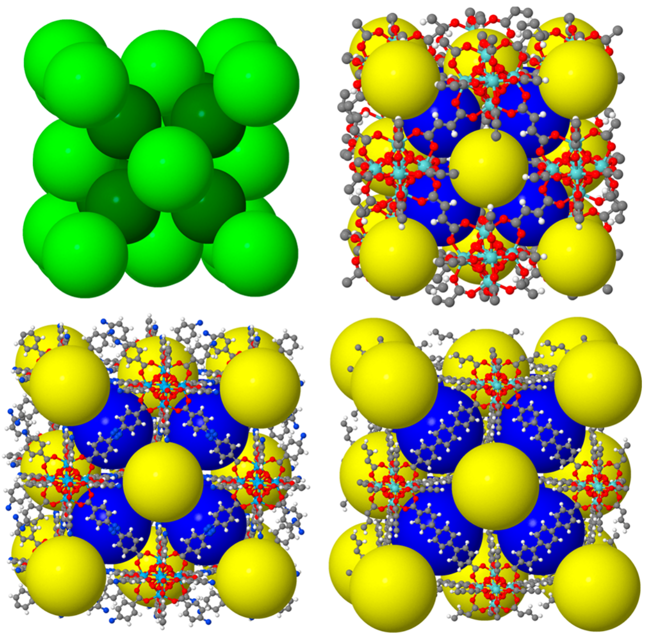

Figure 7. Top left: CaF_2 salt. Top right: MOF-801 with 8 Å spheres in two types of spaces. Bottom left: SUM-5 with 13 Å spheres in two types of spaces. Bottom right: UiO-68 with 14 Å spheres in two types of spaces.

arrangement of calcium atoms with an interpenetrating simple cubic arrangement of fluorine atoms such that the cubic set sits in the tetrahedral holes of the face-centered cubic set. MOF-801,[38] SUM-5,[39] and UiO-68[40,41] have two sets of pores with the same arrangement as does UiO-66[40] shown in the graphical abstract. In the cubic ZnS (zinc blende or sphalerite) structure in Figure 8, half the tetrahedral positions are vacant.

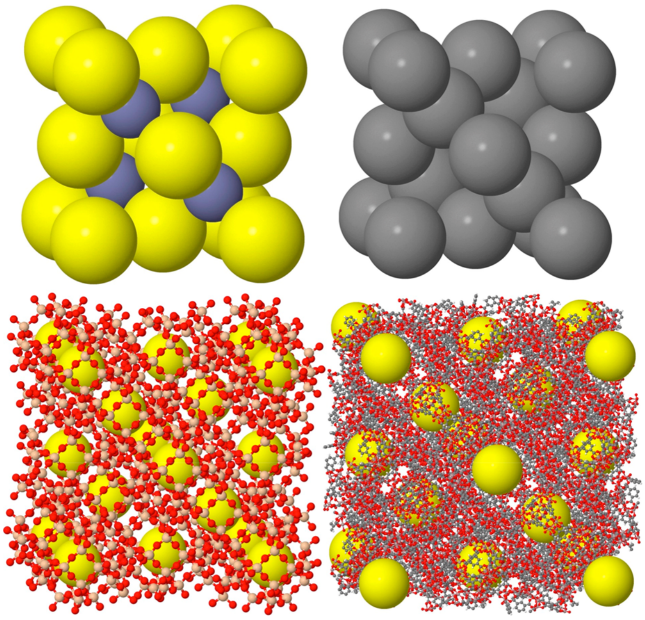

Figure 8. Top left: Cubic ZnS (zinc blende or sphalerite). Top right: Diamond. Bottom left: Faujasite (Zeolite Y) with 6 Å spheres in the spaces. Bottom right: MIL-100 with 16 Å spheres in the spaces.

When both atoms are the same this is the diamond structure. Faujasite (Zeolite Y)[30] and MIL-100[42,43] are framework structures with the diamond arrangement of pores. Over 20,000 atoms are included in Figure 8 for MIL-100, but the diamond structure of the holes can still be identified, clearly illustrating the simplification of looking at the voids as well as the atoms.

■ TOPOLOGY

Another way to simplify framework structures is by topology, viewing the structures as connected links and vertices.[44,45] The vertices could be single atom points or larger units such as polynuclear metal oxide clusters. The points at which such clusters connect to other building units are called points-of-extension. In the carboxylate MOFs, the carboxylate carbon atoms are chosen as the points-of-extension. The links have more than one carboxyl group that attaches to the vertices, and therefore, the points-of-extension define the geometric unit and its overall connectivity in a MOF structure. Topology allows researchers to imagine a structure of a specific connectivity of building units, identify the molecules representing such units, and to build the corresponding structures from those molecules. Often the link is chosen to impart specific length and angle relationships between the molecular building units in order to realize a specific MOF structure. Figure 9 shows examples of 4, 6, 8, and 12 connection vertices. Figure 10 shows examples of linear, trigonal, square, and tetrahedral links.

Network topology nomenclature is an extension of stereochemical nomenclature such as *cis*, *trans*, *fac*, and *mer* for molecular compounds.[46] Different topologies are referred to by three letter names defined by the Reticular Chemistry Structure Resource, RCSR.[47] While *pcu* is primitive cubic, *fcu* is face-centered cubic, *dia* is diamond, and some codes come from mineral names, most topology codes are randomly assigned.[45]

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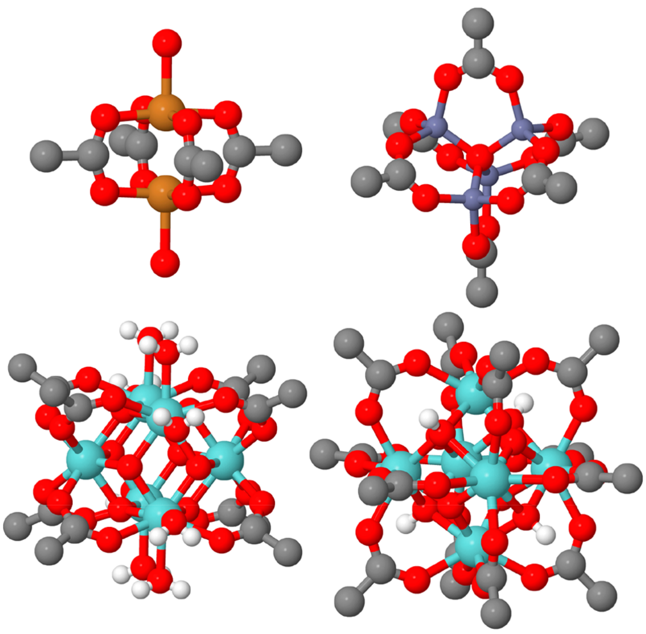

Figure 9. Examples of MOF vertices with carboxylate linkers. Top left: $Cu_2O_2(RCO_2)_4$ with four vertices. Top right: $Zn_4O(RCO_2)_6$ with six vertices. Bottom left: $Zr_6O_8(H_2O)_8(RCO_2)_8$ with eight vertices. Bottom right: $Zr_6O_4(OH)_4(RCO_2)_{12}$ with 12 vertices.

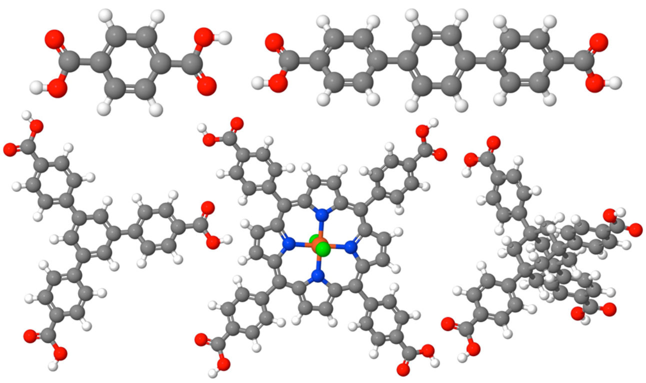

Figure 10. Examples of links with linear, trigonal, square, and tetrahedral shapes.

■ MULTIPLE REPRESENTATIONS

Interactive versions of all figures in this paper are available online,[48] displayed using JavaScript and JSmol[49] without requiring software installation. More experienced chemists make use of a greater variety of representations and visualizations,[50] but there is a need for greater scaffolding in learning such skills.[51] Using computer drawn images where the representation is controlled by the user and can be immediately switched to the same view in another representation provides experience using multiple representations.[52] For example, while the space filling view more accurately shows the atom sizes, chemists routinely use a ball and stick or even a line representation to make the structure less crowded. The cited web page also makes available an interactive slider to control the size of spheres located in the structure pores. See Figure 11. This facilitates comparing pore sizes in different structures, as illustrated in Figures 1−8. When highlighting topology, the line representation is useful and showing the metal polyhedra makes the hubs more noticeable

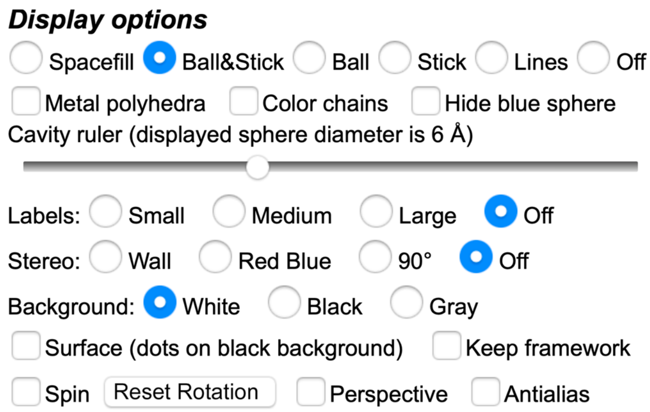

Figure 11. Display options for figures from refs 48, 53, 57.

as seen in Figures 12 and 13. The chain representation is helpful for interpenetrating structures.

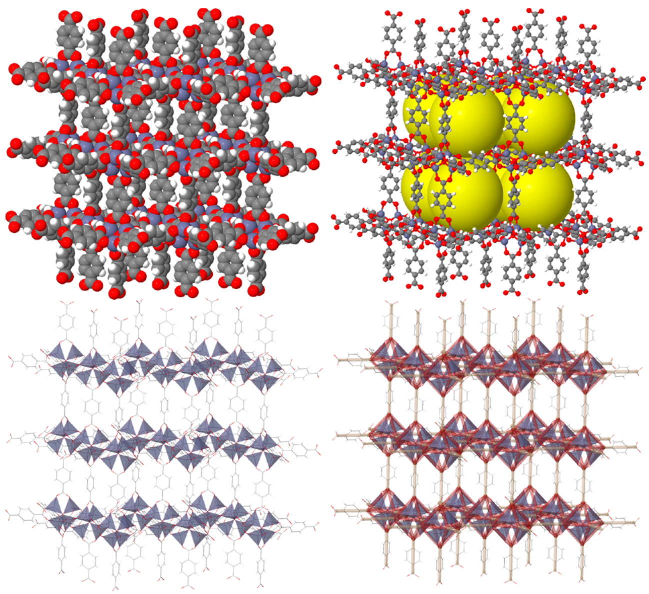

Figure 12. Multiple representations for the same view of IRMOF-1.[29] Top left: Space filling. Top right: Ball and stick with filled pores exhibiting the primitive cubic structure. Bottom left: line drawing with metal polyhedra. Bottom right: line drawing with connectivity.

Ref 48 can be used to interactively illustrate the main concepts in this paper. A typical flowpath on the web page would be to select a structure, wait a few seconds for the coordinates to load, and then drag on the atoms to rotate the structure. In the display options at the bottom of the page, drag on the cavity ruler to populate the pores and adjust the size of their blue and yellow spheres. The two colors represent crystallographically independent pores. Select spacefill, ball and stick, or lines to represent the atoms and better see the blue and yellow spheres. Identify the blue and yellow spheres as matching a simple structure. To examine the framework topology you might then select metal polyhedra as a display option and/or click on the radio button in front of the three letter topology code next to the structure name. (Clicking on the code itself goes to the RCSR topology database.)

An additional web page[53] is available to examine the structures and show just the link, just the vertex, each type of pore, or the framework. The additional page has the same

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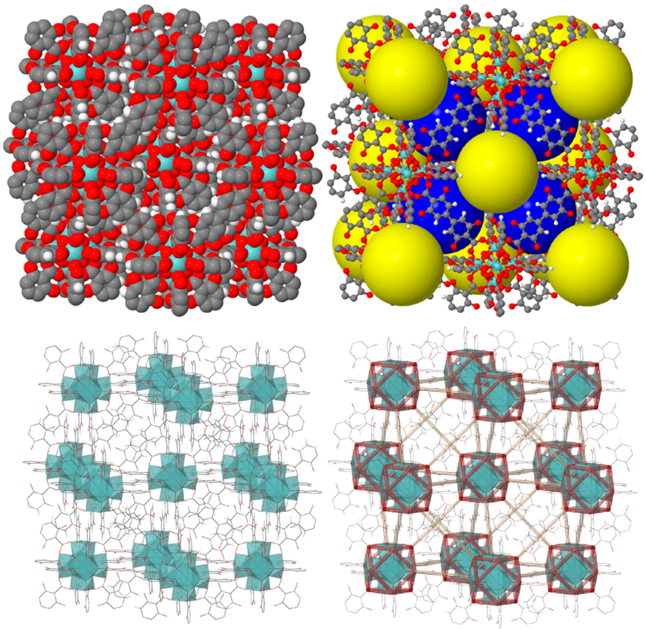

Figure 13. Multiple representations for the same view of MOF-806.[38] Top left: Space filling. Top right: Ball and stick with filled pores exhibiting the fluorite structure. Bottom left: line drawing with metal polyhedral. Bottom right: line drawing with connectivity.

controls as in Figure 11, a larger selection of MOFs, is better suited toward measuring pore size but does not include the comparisons with simple structures.

■ STUDENT LEARNING

The above material was introduced after a session that used physical model kits[54−56] to build the primitive cubic, body-centered cubic, face-centered cubic, CsCl, NaCl, fluorite, zinc blende, and diamond structures. The material was presented in the spirit of extending what students had previously learned to a new and important area of chemistry and as a check to see if students could recognize the cubic structures. Students were asked to identify the structure of the MOF pores using a web page that did not include the answers.[57] A third of the students correctly identified all of the structures, but another third of the students only identified a few structures. A discovered misconception was that a substantial number of students thought the CsCl structure was body-centered cubic; this was then discussed further in the next class. Students did seem to appreciate the addition of applications and current research to the model building exercise.

With additional time and possibly working in pairs, students can (1) imagine a net, (2) deconstruct it into its vertices and links constituents, and then (3) select molecules such as those in Figures 9 and 10 that correspond to the geometries of those constituents.[44,45]

■ SUMMARY

Models are used to simplify complex phenomena, and molecular models often have the goal of reconstructing a three-dimensional object in your mind.[58] Making connections between known cubic structures and pore locations, identifying the topology of connected links and vertices, and using multiple representations can be powerful simplifications for visualizing MOFs.

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Notes

The authors declare no competing financial interest.

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(26) While structure names suggest a specific compound, the formulas represent structural types. For example, the NaCl structure is exhibited by AgBr, AgCl, AgF, BaO, BaS, BaSe, BaTe, CaO, CaS, CaSe, CaTe, CdO, CoO, CrN, CsF, CsH, KBr, KCl, KF, KH, KI, LiBr, LiCl, LiF, LiH, LiI, MgO, MgS, MgSe, MnO, MnS, MnS, NaBr, NaCl, NaF, NaH, NaI, NbC, NbO, NiO, PbS, PbSe, PbTe, PdH, RbBr, RbCl, RbF, RbH, RbI, ScAs, ScN, ScSb, SnAs, SnSb, SnSe, SnTe, SrO, SrS, SrSe, SrTe, TaC, TaO, TiC, TiN, TiO, VC, VN, YAs, YN, YTe, ZrB, ZrC, ZrN, ZrO, ZrP, and ZrS; the ZnS sphalerite or zinc blende structure is exhibited by AgI, AlAs, AlP, AlSb, BAs, BN, BP, BePo, BeS, BeSe, BeTe, CdPo, CdS, CdSe, CdTe, CuBr, CuCl, CuF, CuI, GaAs, GaP, GaSb, HgS, HgSe, HgTe, InAs, InP, InSb, MnS, MnSe, SiC, ZnPo, ZnS, ZnSe, and ZnTe; the CaF_2 fluorite or fluorspar structure is exhibited by $AuAl_2$, $AuGa_2$, $AuIn_2$, $AuSb_2$, $BaCl_2$, BaF_2, Be_2B, Be_2C, CaF_2, CdF_2, $CoSi_2$, $GeMg_2$, HfO_2, HgF_2, $IrSn_2$, Ir_2P, K_2O, K_2S, K_2Se, K_2Te, Li_2O, Li_2S, Li_2Se, Li_2Te, Na_2O, Na_2S, Na_2Se, Na_2Te, NbH_2, $NiSi_2$, β-PbF_2, $PbMg_2$, α-PoO_2, $PtAl_2$, $PtGa_2$, $PtIn_2$, $PtSn_2$, RaF_2, Rb_2O, Rb_2S, Rb_2P, ScH_2, $SiMg_2$, SmH_2, $SnMg_2$, $SrCl_2$, SrF_2, YH_2, and ZrO_2; and the CsCl structure is exhibited by CsBr, CsI, RbCl, ThTe, TlBr, TlCl, TlI, AgCd, AgCe, AgLa, AgMg, AgZn, AlNd, AlNi, AuCd, AuMg, AuZn, BeCo, BeCu. BePd, CdCe, CdLa, CdPr, CuZn, LiAg, LiHg, LiTl, MgCe, MgHg, MgLa, MgSr, CaTl, MgTl, and SrTl.
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