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**Supporting information for article:**

***Model2SAS: a software for small-angle scattering data calculation from custom shapes***

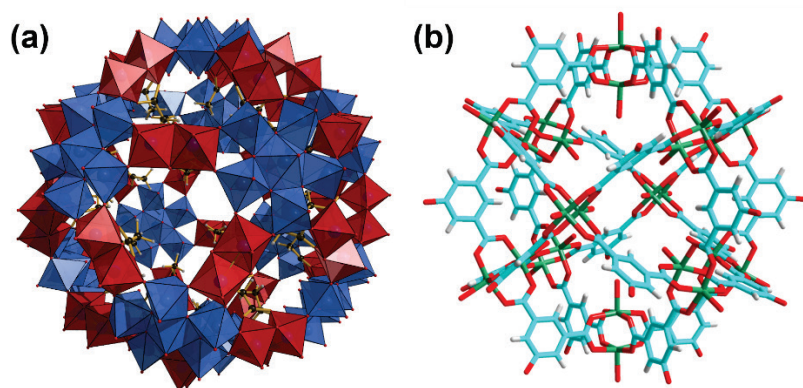
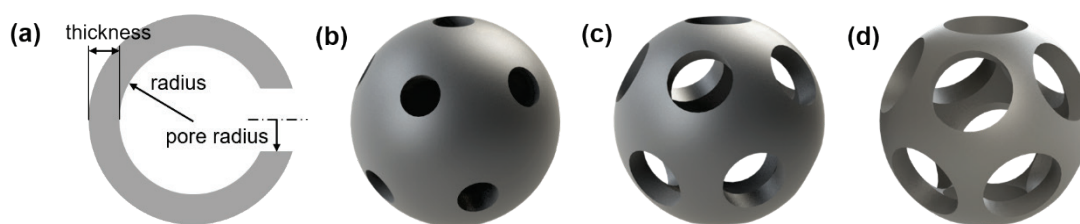
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**Table S1** Parameters of core-2shell model.

Parameter	Core radius	Shell thickness 1	Shell thickness 2	SLD core	SLD shell 1	SLD shell 2
Value	30	5	15	1	3	2

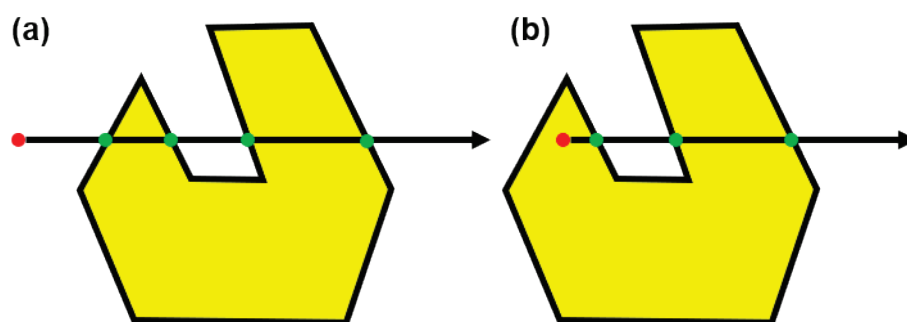
**Table S2** Parameters of cylinder model.

Parameter	Radius	Length	SLD
Value	30	30	1

**Figure S1** (a) A polyhedral model of  $\{\text{Mo}_{132}\}$ ; (b) A stick model of  $\text{Cu}_{24}(\text{5-OH-IPA})_{24}$  MOP.**Figure S2** (a) graphical representation of parameters of porous spherical shell model. And renderings of porous spherical shell models with different pore radius: (b) 2.5, (c) 4, (d) 5.

**Table S3** Parameters of porous spherical shell and corresponding spherical shell.

	Spherical shell	Porous spherical shell 1	Porous spherical shell 2	Porous spherical shell 3
SLD	1	1	1	1
Radius	10	10	10	10
Thickness	2.5	2.5	2.5	2.5
Pore number	-	12	12	12
Pore radius	-	2.5	4	5



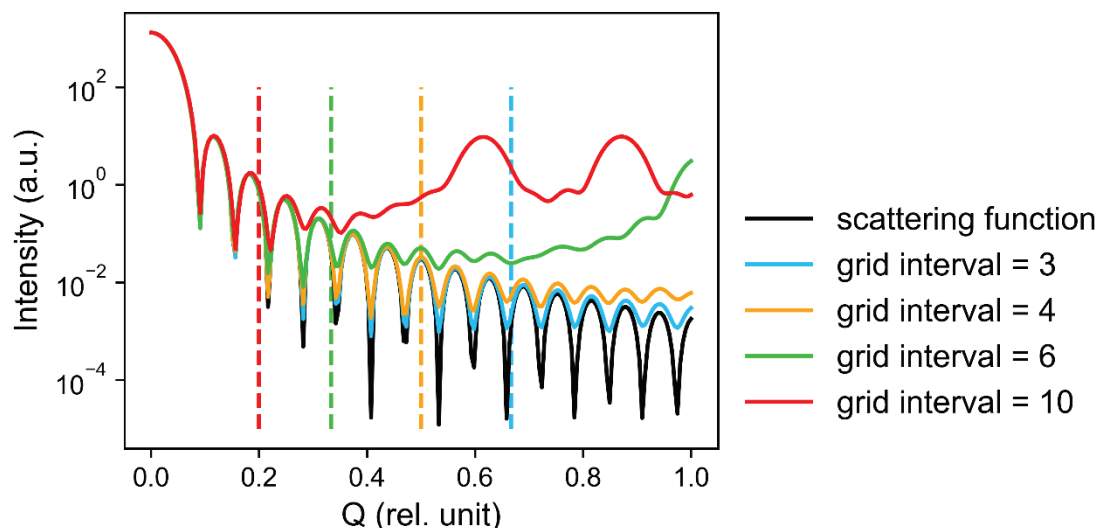
**Figure S3** Scheme of determining whether a point is in a shape or not. Draw a ray with arbitrary direction from a certain point (red point) and count the number of intersection (green points). If number of intersections is even number (e.g. 4 intersection points in (a)) then this certain point is not in the shape (yellow).; If number of intersections is odd number (e.g. 3 intersection points in (b)) then this certain point is in the shape (yellow).

#### S1. The influence of grid density on precision of calculated SAS curve.

Discretization approximation of a shape is valid when length scale much larger than grid interval.

Thus, in reciprocal space, the maximum acceptable  $q$  value should be proportional to  $(\text{interval})^{-1}$ . In

the example of sphere with radius=50, we find that  $\frac{2}{\text{interval}}$  is an appropriate criterion for maximum  $q$  (Figure S4). It must be noted that an acceptable configuration may vary with the complexity of model, computing power, desired precision and  $q$  range required.



**Figure S4** Calculated SAS curves of sphere with radius=50, from both scattering function (black) and models with different grid density (interval of grid points equals to 3 (blue), 4 (orange), 6 (green) and 10 (red) respectively). Q coordinates of dashed lines are  $\frac{2}{\text{interval}}$  of corresponding colour.

## S2. Experimental procedures of MOPs

**Synthesis.** The synthesis followed the literature.(Sun, L.-B.; Li, J.-R.; Lu, W.; Gu, Z.-Y.; Luo, Z.; Zhou, H.-C., Confinement of Metal–Organic Polyhedra in Silica Nanopores. *J. Am. Chem. Soc.* **2012**, *134* (38), 15923-15928.) A solution (10mL) of 5-hydroxy-1,3-benzenedicarboxylic acid (365 mg) in dried methanol was mixed with a solution (30mL) of  $\text{Cu}_2(\text{OAc})_4 \cdot 2\text{H}_2\text{O}$  (400 mg) in dried methanol in a glass vial (50 mL) and stirred for 1 hour at room temperature. Then 10 mL of N,N-dimethylacetamide was added to this solution and then allowed the vial stand at room temperature for several days. Then the precipitates were separated by centrifuge, washed by diethyl ether and dried.

**SAXS.** SAXS measurements were conducted on the beamline 12-ID-B of Advanced Photon Source in the Argonne National Laboratory. The MOP solutions for SAXS measurements are ca. 5 mg/mL methanol solutions loaded in quartz capillary. Background scattering was measured separately with solvents in quartz capillary and subtracted from MOP solution scattering data.