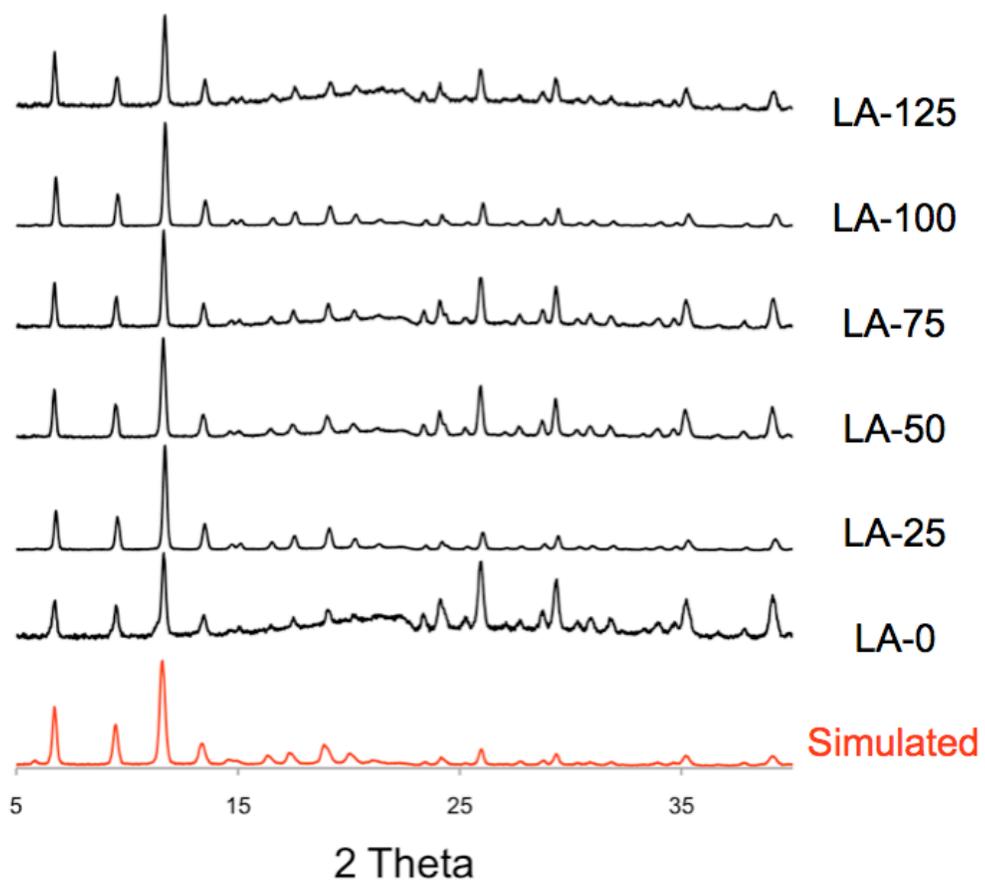


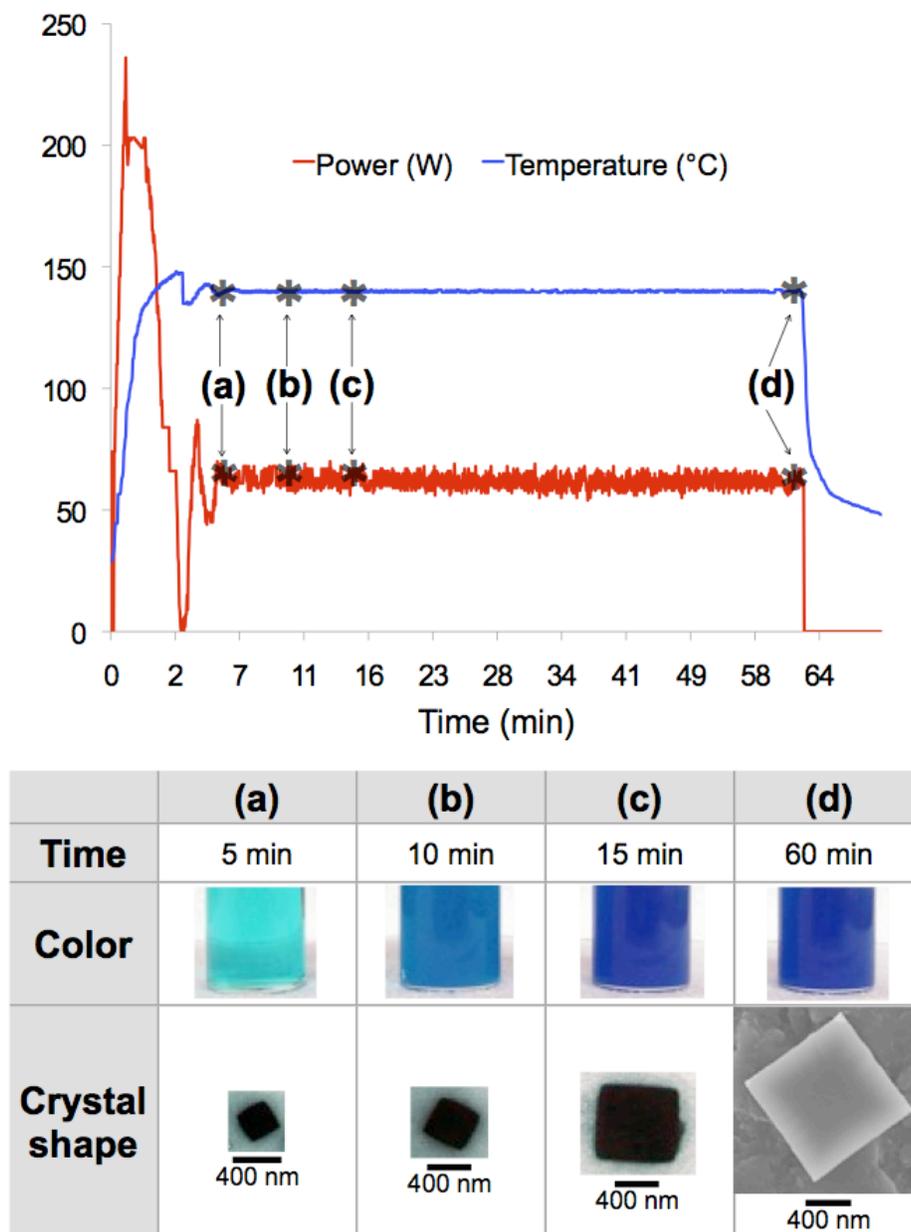
## Supporting Information

# Morphology Design of Porous Coordination Polymer Crystals by Coordination Modulation

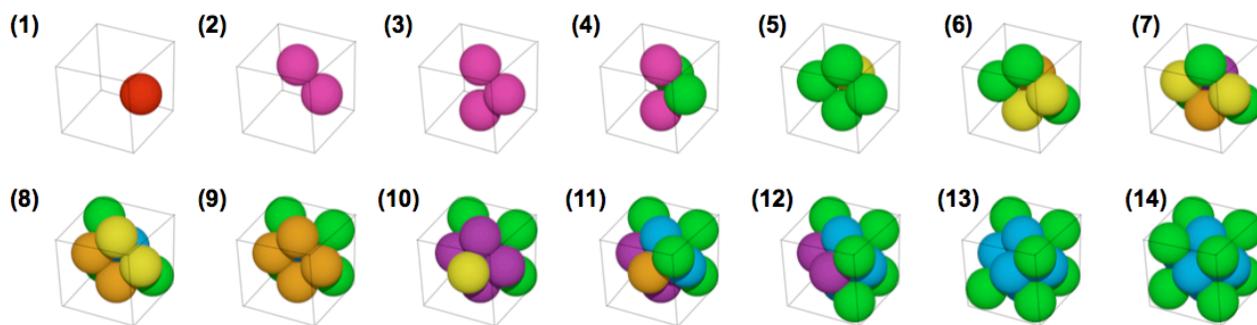
Ayako Umemura, Stéphane Diring, Shuhei Furukawa,\* Hiromitsu Uehara, Takaaki  
Tsuruoka, and Susumu Kitagawa\*



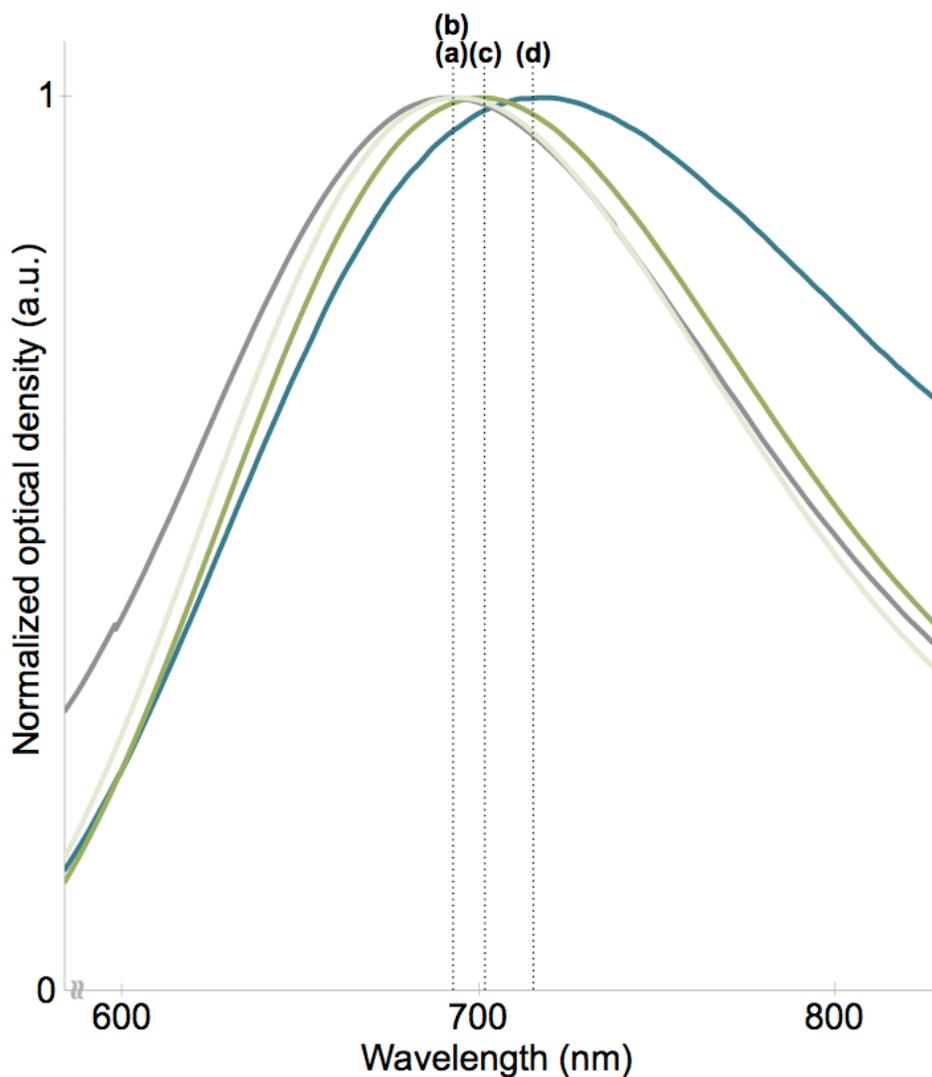
**Figure S1.** X-ray powder diffraction patterns of  $\text{Cu}_3(\text{btc})_2$  synthesized from copper nitrate with LA-0, 25, 50, 75, 100 and 125 and simulated.



**Figure S2.** Time-course observation of  $\text{Cu}_3(\text{btc})_2$  crystal when LA-125. The graph shows a trend of power and temperature on MW machine when the performance was set for 60 minutes at 140 °C. As seen in the inset table, at 5, 10 and 15 minutes with a color shift of solution obtained, TEM images of  $\text{Cu}_3(\text{btc})_2$  crystal shape was confirmed as a cube similarly as seen at 60 minutes. There was neither octahedron nor cuboctahedron observed.



**Figure S3.** In this study, site type definition of the coarse-grain model is described in colors by the number of attached coordination. The attachment progresses in the face-centered cubic network. (1) to (14) shows a series of building a growth unit in the face-centered cubic network. Red, pink, green, yellow, orange, purple and light blue correspond to ZERO, ONE or TWO, THREE (*i.e.* 2D-nucleation on  $\{111\}$  facets as green seen in (14)), FOUR (*i.e.* 2D-nucleation on  $\{100\}$  facets as yellow in (10)), FIVE, SIX and SEVEN or EIGHT (*i.e.*  $\{100\}$  facets as light blue in (14)), respectively. Other bulky sites (*i.e.* NINE to TWELVE) are not shown here, however, they were set as blue ( $\{111\}$  facets).



**Figure S4.** UV-vis spectrum showing the interaction of copper metal sources and *n*-dodecanoic acid (modulator) in butanol. When increasing the concentration of modulator to LA-125, the  $\lambda_{\max}$  of copper acetate (702 nm) also approached the  $\lambda_{\max}$  of copper laurate in butanol (695 nm).  $\lambda_{\max}$  refers to (a) copper laurate (695 nm); (b) copper acetate with LA-125 (695 nm); (c) copper acetate (702 nm) and (d) copper nitrate with LA-125 (720 nm) in butanol.

## Full authors list of reference 11a

(a) Horcajada, P.; Chalati, T.; Serre, C.; Gillet, B.; Sebrie, C.; Baati, T.; Eubank, J. F.; Heurtaux, D.; Clayette, P.; Kreuz, C.; Chang, J.-S.; Hwang, Y. K.; Marsaud, V.; Bories, P.-N.; Cynober, L.; Gil, S.; Férey, G.; Couvreur, P.; Gref, R. *Nature Mater.* **2009**, *9*, 172-178.