

Poster Presentation

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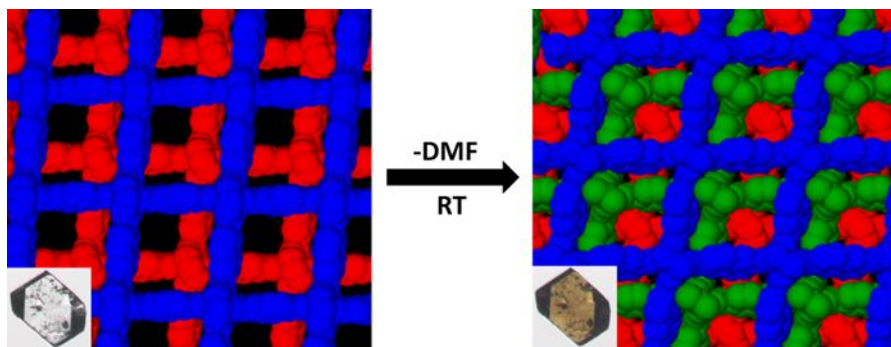
Direct evidence for 2-fold to 3-fold change of interpenetration in a MOF

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Single-crystal to single-crystal transformations has recently received much attention in the field of crystal engineering. Such transformations not only provide insight into the changes taking place within the crystal at the molecular level, but they also aid our understanding of the structure-property relationships. Discrete crystals have been shown to tolerate considerable dynamic behavior at the molecular level while maintaining their single-crystal character. Examples that are common in the literature include bond formation/cleavage,[1] guest uptake,[2] release or exchange as well as polymorphic phase transformations. However, there are rare examples of the structural transformations on the host framework initiated by removal of guest or change in physical conditions such as temperature or pressure. We have investigated a known doubly-interpenetrated metal organic framework with the formula [Zn₂(ndc)₂(bpy)] which possesses minimal porosity when activated. We have shown not only that the material converts to its triply-interpenetrated analogue upon desolvation, but that the transformation occurs in a single-crystal to single-crystal manner under ambient conditions.[3] This contribution probes the limits to which a single-crystal material can undergo structural rearrangement while still maintaining the macroscopic integrity of the crystal as a discrete entity.

[1] M. C. Bernini, F. Gandara, M. Iglesias, N. Snejko, E. Gutierrez-Puebla, E. V. Brusau, G. E. Narda, M. A. Monge, *Chem. Eur. J.* 2009, 15, 4896, [2] T. Jacobs, G. O. Lloyd, J.-A. Gertenbach, K. K. Müller-Nedebock, C. Esterhuysen, L. J. Barbour, *Angew. Chem. Int. Ed.* 2012, 51, 4913., [3] H. Aggarwal, P. M. Bhatt, C. X. Bezuidenhout, L. J. Barbour, *J. Am. Chem. Soc.* 2014, 136,3776



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