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Supporting information for article:

Detailed total scattering analysis of disorder in ZIF-8

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Supplemental Information: Detailed total scattering analysis of disorder in ZIF-8

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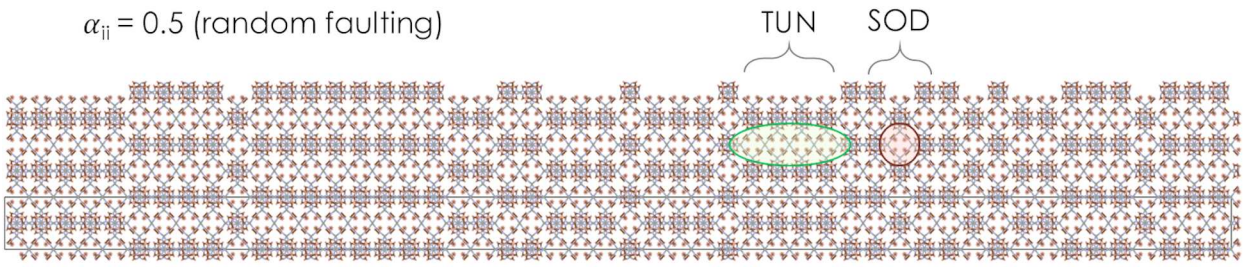
1. Visualization of [001] layer faulting model

In the main text we note that layer models can be selected by "... slicing chemically-sensible bi-periodic slabs of least volume ..." from the crystalline parent structure model.

Because the average structure is unchanged in the model of position fluctuation of layers stacked in the [011] direction, the model is guaranteed to be chemically sensible– i.e. maintain Zn-imidazolate bonding.

The model of faulted layer stacking introduces a new stacking vector, and it is necessary to investigate whether the proposed model maintains sensible connectivity, avoids unphysical bonding, and so on. A projection of this layer model with random faulting is presented in the figure below. The distinctive feature of this model is that it maintains the tetrahedral Zn coordination environment, while introducing a new topology to the extended structure. In contrast to the sodalite (SOD) framework which

features approximately spherical pores, the defective stacking arrangement (R_B = (0 **a**, 0 **b**, 1 **c**)) forms elongated tunnel-like fragments (indicated as "TUN").



. See main text for further description of the model.

Fig. 1. Example of faulting in a ZIF-8 derived ensemble. Normal (sodalite: SOD) ZIF-8 is formed by repeat stacking vectors R_A = ($\frac{1}{2}$ **a**, $\frac{1}{2}$ **b**, 1 **c**). The introduction of the stacking vector R_B = (0 **a**, 0 **b**, 1 **c**) creates non-sodalite fragments (tunnel: TUN)