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Framework defects in microporous materials[1] NICHOLE MAUGHAN, SUMNER NORMAN, DANIEL ROBERTSON, BRANTON CAMPBELL, Brigham Young University — Zeolites are alumino-silicate microporous materials, having three-dimensionally connected frameworks of channels and cavities through which ions and molecules can flow. Because the atomic configuration of such a material strongly affects its useful properties, any defects present in the crystal structure will also impact those properties. Defects break the translational symmetry of a crystal, and thereby transfer scattered intensity out of the compact Bragg reflections and into a continuous but structured diffuse background, which appears as fuzzy streaks in CCD x-ray scattering images. Several zeolite analogs with the AFI framework type exhibit strong diffuse scattering patterns in addition to the expected Bragg scattering, leading us to believe that its framework structure is prone to topological defects. We are working to characterize these defects using single-crystal diffuse scattering data. We have generated a number of candidate defect models and calculated their corresponding diffuse scattering patterns in order to compare them against the experimental data. Ultimately, we aim to find an atomistic-defect model that accurately that explains the data.

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