Abstract Submitted for the 4CF11 Meeting of The American Physical Society

Defect-induced diffuse scattering in microporous aluminophosphate-5 NICHOLE M. MAUGHAN, Brigham Young University, SUMNER NORMAN, Department of Mechanical Engineering, University of Utah, DANIEL G. ROBERTSON, BRANTON J. CAMPBELL, Department of Physics and Astronomy, Brigham Young University — Microporous framework materials, the most common type being aluminosilicate zeolites, are crystalline compounds with interconnected networks of channels and cavities through which ions and molecules can flow. Aluminophosphate-5 (AlPO-5) is a zeolite analog in which alternating aluminum and phosphorus atoms occupy the tetrahedral sites of the AFI framework type. AlPO-5 is useful as a molecular sieve, especially when doped with chromium. Our single-crystal X-ray diffuse scattering (SCXDS) data from AlPO-5 reveals evidence of planar framework defects that have the potential to alter the material's useful properties. By generating candidate defect models, simulating their diffuse scattering patterns, and comparing them against experimental data, we aim to establish the correct model.

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