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Entropic inflation of ideal zeolitic frameworks VITALIY KAPKO, COLBY DAWSON, MICHAEL TREACY, Arizona State University — Ideal zeolites can be viewed as flexible networks of rigid, corner-sharing tetrahedra. Recent studies have shown that such systems can exist at a range of densities (termed the "flexibility window") without breaking topology or deforming the comprising tetrahedra. They also have shown that densities of real zeolites almost always correspond to the lowest densities within this range. This anomalous behavior is usually attributed to coulombic repulsion between oxygen atoms in framework cavities and channels. In this paper we show that the inflation of ideal zeolites can be driven by entropy. This effect is closely related to displacive phase transitions often observed in zeolites and related materials like quartz, which cannot be explained by potential energy minimization alone. We show that periodicity and high symmetry in ideal zeolites is a result of entropy maximization. An estimation of entropy using a harmonic oscillator model with a realistic force field is given.

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