Abstract Submitted
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**Flexibility of zeolite frameworks** VITALIY KAPKO, MICHAEL TREACY, MICHAEL THORPE, Department of Physics Arizona State University — Zeolites are an important class of industrial catalysts because of their large internal surfaces and molecular-sieving properties. Recent geometric simulations (1) show that almost all of the known zeolites can exist without distortion of their tetrahedra within some range of densities, which we call the flexibility window. Within this window, the framework accommodates density changes by rotations about the shared tetrahedral corners. We argue that the presence of a flexibility window can be used as a topological criterion to select potential candidates for synthesis from millions of hypothetical structures. We also investigate the exceptions to the rule, as well as the shape of the flexibility window and the symmetric properties of zeolites inside it. (1) A. Sartbaeva, S.A. Wells, M.M.J. Treacy and M.F. Thorpe The flexibility window in zeolites, Nature Materials 5, 962-965 (2006); I. Rivin, commentary 931-932.

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