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Michael W Deem* (mwdeem@rice.edu), 6100 Main Street - MS 142, Houston, TX 77005. *A Database of Computationally-Predicted Zeolite-Like Materials.*

We here describe a database of computationally predicted zeolite-like materials. These crystals were discovered by a Monte Carlo search for zeolite-like materials. Positions of Si atoms as well as unit cell, space group, density, and number of crystallographically unique atoms were explored in the construction of this database. The database contains over 2.6M unique structures. Roughly 15% of these are within +30 kJ/molSi of alpha-quartz, the band in which most of the known zeolites lie. These structures have topological, geometrical, and diffraction characteristics that are similar to those of known zeolites. The database is the result of refinement by two interatomic potentials that both satisfy the Pauli exclusion principle. The database has been deposited in the publicly available PCOD database and www.hypotheticalzeolites.net/database/deem/. (Received August 09, 2011)