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The flexibility of zeolites for Hydrogen storage ASEL SARTBAEVA, Oxford University, STEPHEN ANTHONY WELLS, Warwick University, PETER P. EDWARDS, Oxford University — The flexibility window is a newly discovered theoretical measure which can provide a valuable selection criterion when evaluating hypothetical zeolite framework structures as potential synthetic targets. Today synthetic zeolites are the most important catalysts in petrochemical refineries. There have been considerable efforts to synthesize new zeolites with specific pore geometries, to add to the 167 available at present. Millions of hypothetical structures have been generated on the basis of energy minimization, and there is an ongoing search for criteria capable of predicting new zeolite structures. The flexibility window appears to be a property of existing zeolite frameworks not shared by many hypothetical structures. It provides a valuable selection criterion when evaluating hypothetical zeolite framework structures as potential synthetic targets. We are investigating the use of zeolites as hydrogen storage materials, as small molecules such as molecular hydrogen and ammonia can be easily absorbed into a flexible framework of zeolites. An exiting possibility is the use of framework flexibility to control hydrogen uptake, storage and release. This would allow a safe use of hydrogen for fuel cells.

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