Shape Selective Catalysis and Separation

James Wei

Princeton University, Princeton, NJ

ABSTRACT

Design of shape selectivity in catalysis is traditionally carried out by comparison of the molecular diameters with the window diameters, which is acceptable with roughly spherical molecules and circular windows. However most molecules in solution are closer to an ellipsoid than to a sphere, characterized by a length L, and two diameters D_1 and D_2. A more rational design procedure is to characterize each window and each molecule by the major and minor diameters, to determine entry possibility. However all molecules are flexible and can be squeezed to enter a window that is 10-20% smaller, especially at elevated temperatures.

We have developed a computational method, and calculated the strain energy involved in squeezing a given molecule into a given window. We have also developed a database with 280 molecules and 220 zeolite windows, which can be used to design separation processes.

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