

# Designing zeolites for catalytic applications

Avelino Corma

*Instituto de Tecnología Química*

Different zeolite synthesis concepts have resulted in a better understanding of the synthesis mechanisms and in the development of new structures and applications. From the point of view of the zeolitic catalysts, previous knowledge and intuition allows to select, among different structures, those that may be useful to catalyse a certain reaction. The main criteria of selection is based on pore dimensions and pore topology. Then, when a first selection has been made, further improvements can be achieved by adapting chemical composition and crystallite size.

There is no doubt that it would be desirable to directly synthesize a zeolite that fulfils the geometrical requirements for a given reaction, while locating the active sites at the required framework position, in such a way that an optimum matching between the zeolite and the reaction transition state will be established. This should drive into a minimization of the activation energy of the process and, specially, a maximization of the selectivity to the desired product.

Besides discussing synthesis methods for preparing new zeolites, based on former concepts, and showing their possibilities for adsorption/separation and catalysis, a methodology for the “a priori” synthesis of zeolites directed to specific applications will be presented. Within this methodology, a reaction mechanism for the catalytic process is first postulated, that includes a potential reaction transition state. Then, a mimic of such a transition states (TS) is synthesized as Organic Structure Directing Agent (OSDA) and the zeolite synthesis is carried out certainly using previous existing knowledge on the influence of gel composition time and temperature, for performing the synthesis. The methodology not only should be useful for directing into structures with pores and cavities adapted for reaction TS stabilization, but also should direct the location of framework charge compensation for a given catalytic reaction.

It will be shown that, following the above methodology, it is possible to prepare zeolites with improved activity and selectivity than the ones used today for chemical and petrochemical processes during alkylaromatics transformations, and for cracking processes directed to maximize olefins productions.