Rational Design of Zeolites for Catalysis: Myth or Reality?

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Chemistry relies on the design and control of systems over multiple-length scales ranging from the molecule to the crystal [1]. The assembly at the molecular level involves at least two species, based on non-covalent interactions (hydrogen bonding, electrostatic forces, van der Waals forces, metal-ion coordination), being the cornerstone of long-range organization [2,3]. Though covalent bonding prevails in zeolites, the latter are meta-stable materials, being produced after successive meta-stable steps [4]. The rational design of zeolites for a targeted reaction frequently remains a challenge that limits its industrial production and application. In this regard, zeolites synthetized via two independent strategies were investigated: (i) the 'fluoride route' revisited giving rise to (almost) perfect giant crystals [5]; (ii) the use of biomass residues to guide the zeolite nanocrystals self-assembly [6].

Both catalysts have demonstrated *good* to *outstanding* performances and selectivities in the reaction of methanol-to-hydrocarbons, either producing light olefins or gasoline fraction. The effect of different synthesis parameters modification on zeolite crystallinity, acid site density, crystal size and morphology has been investigated 'in-depth' and correlated with the data acquired from acid catalysis.

Though those results appear promising, one still has to bridge the gap between the potential at lab-scale and future industrial implementation, while overcoming issues related to shaping, mass transfer, process safety, economics and geopolitics.





Figure. SEM images of ZSM-5 zeolite crystals obtained via biomass-templated route (left); fluoride mediated route (right)

References

[1] J.M. Lehn, Science 1985, 227, 849.

[2] G.M. Whitesides, B. Grzybowski, Science 2002, 295, 7378.

[3] P. Mothe-Esteves, M. M. Pereira, J. Arichi, B. Louis, Cryst. Growth Des. 2010, 10, 371.

[4] S. Mintova, M. Jaber, V. Valtchev, Chem. Soc. Rev. 2015, 44, 7207.

[5] P. Losch, A.B. Pinar, M.G. Willinger, K. Soukup, S. Chavan, B. Vincent, P. Pale, B. Louis, *J. Catal.* **2017**, 345, 11.

[6] M.M. Pereira, E.S. Gomes, A.V. Silva, A.B. Pinar, M.G. Willinger, S. Shanmugam, C. Chizallet, G. Laugel, P. Losch, B. Louis, *Chem. Sci.* **2018**, 9, 6532.