We have proposed the charge stabilization index, CSI\(^i\), models often lead to conflicting predictions.\(^2\) The well established stability rules for neutral fullerenes, such as isolated-pentagon rule (IPR), are not always valid for charged fullerenes. An unusual behavior of charged fullerenes is that the isomer relative stability could be substantially different from that of their neutral counterparts.\(^1\) The power of CSI has been systematically checked by considering all fullerene isomers from C\(_{28}\) to C\(_{104}\) with charges between +6 and –6. The model correctly predicts the structures observed experimentally and those determined by geometry optimizations nor iterative electronic structure calculations, but just the knowledge of cage connectivity.

In this presentation, we propose a simple and general scheme\(^3\) based on the concepts of cage connectivity and frontier \(\pi\) orbitals that allows to fully understand the stability of both anionic and cationic fullerenes. It needs neither aromaticity and the minimum electrostatic repulsion, have been proposed for fullerene anions.\(^2\) However, these approximations are no longer valid for many experimentally observed structures. Which are then the underlying rules that govern the stability of charged fullerenes? Some approximate rules, based on different physical arguments, such as maximum aromaticity and the minimum electrostatic repulsion, have been proposed for fullerene anions.\(^2\) However, these rules are not always valid for charged fullerenes. The well established stability rules for neutral fullerenes, such as isolated-pentagon rule (IPR), are not always valid for charged fullerenes. An unusual behavior of charged fullerenes is that the isomer relative stability could be substantially different from that of their neutral counterparts.\(^1\) The power of CSI has been systematically checked by considering all fullerene isomers from C\(_{28}\) to C\(_{104}\) with charges between +6 and –6. The model correctly predicts the structures observed experimentally and those determined by geometry optimizations nor iterative electronic structure calculations, but just the knowledge of cage connectivity.

The increasing demand of light olefins in the industry has renewed interest of the methanol-to-olefins process (MTO) as a route to obtain these petrochemicals from sources alternative to petroleum\(^1\). Some zeolitic nanoporous silicoaluminophosphates, such as SAPO-35, are active catalysts in the MTO process, raising selectivities to light olefins up to 80%. The main drawback of this catalyst in the MTO process is its rapid deactivation caused by the deposition of bulky molecules in the pore entrances and the external surface, which blocks the accessibility of the reactants to the active acid sites and the diffusion of products out of the nanopores. However, the deactivation can be restrained by modifying properly the synthesis conditions of the catalysts in order to obtain crystals with improved properties. Textural properties as well as crystal size are key parameters to enhance the stability of these kind of catalysts in the MTO process\(^2-3\).

In this sense, we have used glucosamine as additive in the synthesis of SAPO-35 (framework type LEV) and found that it provokes an important reduction of crystal size. It is postulated that the crystal growth modifier effect of the glucosamine can be triggered by the \(-\text{NH}_2\) group of the glucosamine molecules present in the synthesis gel, that can interact with SAPO-35 nuclei, surrounding them and inhibiting their growth. The synthesis of SAPO-35 under controlled conditions also favours the formation of regular cubic crystals instead of macle ones. Furthermore, it was found that the observed outcome was strongly dependent on the percentage of glucosamine added to the synthesis gel. Crystal size decreased rapidly as glucosamine concentration increased up to 0.5% but, at higher concentrations, size reduction was progressively lower as the percentage of glucosamine added to the synthesis gel increased. Thus, it was possible to obtain SAPO-35 nanoporous catalysts with a directed crystal size.

As it is well known that crystal size is a key factor determining the deactivation of these catalysts in the MTO process, this method allows to obtain catalysts with improved stability under reaction conditions (Test conditions: WHSV=1.2h\(^{-1}\), T=400ºC).

**Notes and References**