COMBINING THEORY AND EXPERIMENT, AN X-RAY ABSORPTION SPECTROSCOPY STUDY ON IRON POLYMERIZATION CATALYSTS

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In the late 90's, a very active iron-based ethylene polymerization catalyst was discovered, the process was improved by the use of methylalumoxane (MAO) as activator. Although good iron catalysts for ethylene polymerization are known, the exact mechanism of olefin polymerization and the determination of whether MAO activation of the precursor forms iron (II) or iron (III) species remains under discussion.

In order to answer these questions, we applied X-ray absorption spectroscopy, a very powerful tool in material science, as it probes the electronic and geometrical structures around the absorbing atom. The so called 'freeze-quench' XAFS methodology that we developed allows for 'trapping' of the active species in various stages of pre-activation and catalysis, by rapid freezing of the catalyst solution. In this part of the project I have focused on the computational modelling of possible intermediates, and even their corresponding X-ray absorption spectra, in order to understand the activation mechanism completely.