

**DIPLÔME NATIONAL DE DOCTORAT**

**(Arrêté du 25 mai 2016)**

Date de la soutenance : **20 novembre 2018**

Nom de famille et prénom de l’auteur : **GUTIERREZ ACEBO Ester**

Titre de la thèse : « Impact de la topologie de la structure zéolithique sur le mécanisme et la sélectivité de l’isomérisation bi-fonctionnelle de l’éthylcyclohexane : intégration de l’expérimentation, du calcul ab initio et de la modélisation cinétique multi-échelle  échelle / Impact of the topology of the zeolite structure on the mechanism and selectivity of ethylcyclohexane bifunctional isomerization : experiments, ab-initio calculations and multi-scale kinetic modelling ».



**Résumé**

The paraxylene (pX), used in the manufacture of terephtalic acid for the production of nylon, is mainly produced by isomerization of the C8 aromatic cut. The latter is mainly composed of the three xylene isomers (para, ortho and meta) and ethylbenzene (EB). EB is converted into xylenes by mean of a bifunctional catalyst comprising both an acid function, such as EU-1 zeolite, and a hydro-dehydrogenating function (HD / DHD), such as platinum. The hydrogenation of EB also leads to the production of ethylcyclohexane, which can undergo undesired ring-opening and cracking reactions on the acid function of the catalyst. In this work, we tried to understand the factors influencing the selectivity of the bifunctional catalyst in the hydroconversion of ethylcyclohexane (ECH), and to identify very selective zeolitic acid phases. The effect of parameters such as the ratio and proximity between acid and HD / DHD sites, the location of acid sites within the zeolite network, and the topology of this zeolite network, was evaluated. Catalytic studies have been carried out over bifunctional catalysts series based on the EU-1 zeolite, and interpreted considering ab initio calculations focused on the isomerization and ring-opening mechanisms of ECH on the EU-1 acid phase. The integration of thermokinetic data (determined by ab initio calculations) in a mean field kinetic model made it possible to validate the approach and to identify the key reaction steps dictating the selectivity. A rational screening of zeolite structures was then proposed to identify the influential topological parameters.