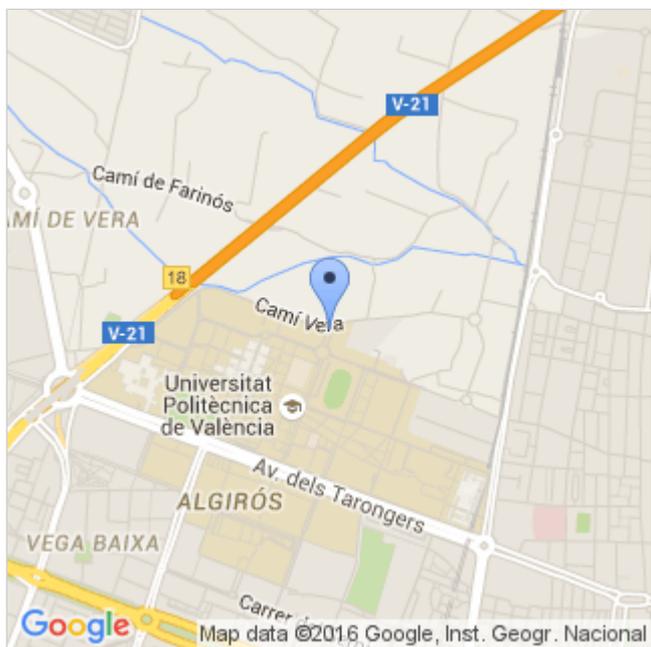


Expression of Interest



Contact Person/Scientist in Charge

- **Name and surname:** German Sastre
- **Email:** gsastre@itq.upv.es

Universitat Politècnica de València (UPV)

Department / Institute / Centre

- **Name:** Instituto de Tecnología Química UPV-CSIC
- **Address:** Campus de Vera, Camino de Vera, s/n, 46022 Valencia
- **Province:** Valencia

Research Area

- Chemistry (CHE)

Brief description of the institution:

Universitat Politècnica de València (UPV) is the single Spanish Technical University that features in the main University world rankings. It is within the top 5 Spanish Universities with the highest revenue from both public research and knowledge transfer activities, and a national leader in patent license income and start up creation. Constituted in 1971, it comprises nearly 30.000 students, over 2500 academics, and 17 university research centres of excellence.

UPV has a relevant experience in the participation in international research programmes, with over 100 FP7 projects and 40 H2020 projects in the period 2014-2015. UPV researchers are also actively involved all H2020 life program stages, from workprogramme drafting discussions, to project coordination. It is also taking part in several major partnering initiatives (JTIs, PPPs, KICs...).

Brief description of the Centre/Research Group (including URL if applicable):

Today, ITQ carries out a very active, intense and successful research on catalysis, photochemistry and material science, transferring the generated knowledge to industry. This spirit has been appreciated by our

colleagues and companies through a number of I+D projects developed jointly with industries and large number ITQ patents, being more than 14 commercially exploited by various companies. However, we are well aware that fundamental research at a molecular level is at the core understanding of chemical processes and the interaction of reactants with catalytic centers. Therefore, we have always been committed to generate that fundamental knowledge.

More information can be found in our recently celebrated 25th Anniversary, where I do recommend to see the programme of lectures: if you enjoy these topics, then ITQ is a good option for you:

<http://www.25anniversaryitq.com/program.html>

Project description:

Searching for suitable zeolites for petrochemical applications using classic molecular dynamics

The present project requires a computational chemist with interest in solid state science. Molecular dynamics is a very suitable technique which will be massively used to try to unveil the diffusional features of hydrocarbon molecules inside the micropore space of zeolites. Zeolites are a large and growing family of crystalline and microporous alumino-silicates whose structures can be visualised here:

<http://izasc.ethz.ch/fmi/xsl/IZA-SC/ft.xsl>.

It happens that although more than 200 structures have been synthesised, many more are possible and there is a hot interest in synthesis methods that allow to synthesise structures with optimum pore-sizes so that the products of certain chemical reactions can be selectively tuned by such pore architecture. Petrochemical reactions, such as those aiming at the selective production of paraxylene are industrially catalysed by 'old-zeolites' and the optimisation of new zeolites could help to improve existing results. The diffusivity of each possible product in the channels of new structures will be explored with molecular dynamics techniques.

Applications

CV and letter of motivation