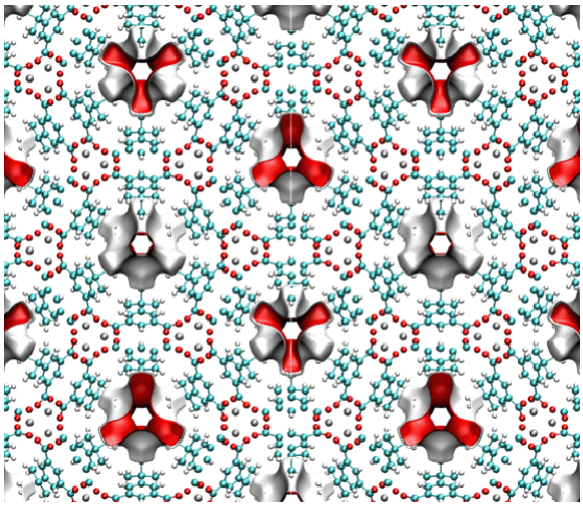
Towards more efficient materials for technological processes (RASPA)



Resumen:

The project is supported by the European Research Council through an ERC Starting Grant.

The RASPA project will provide new insights for material design with a computational investigation of adsorption and diffusion processes in porous materials.

Objetivos:

The key objectives of this research are to:
• Acquire knowledge on the molecular aspects of selective adsorption in porous materials by means of a combination of computational methods.
• Study the interactions between the adsorbates and the adsorbents.
• Understand the effect exerted by changes on the geometry of the material.
• Understand the effect exerted by the chemical composition of the material.
• Define general design guide lines based on the obtained knowledge.

Objectivos contribución:

Dr. Calero's current research focuses on molecular simulations in confined systems. She works with materials used as catalysts and/or adsorbents. As a theoretical and computational chemist, she has developed new force fields and classical simulation approaches for studying adsorption, diffusion, and reaction in porous materials, as well as the growth of materials themselves.

Entregables:

Current research on new porous materials goes beyond just improving established storage, separation, and catalysis. An on-going challenge is to combine methods to adequately integrate diffusion, adsorption, and reaction kinetics. This will lead to the prediction of properties of new high-performance materials with increasing efficiency and speed. The microscopic information that it is planned to be obtained from this project provides the underlying knowledge from a molecular point of view that may guide to the development of more efficient processes, to fine-tune materials for a particular application, and also to steer the experimental effort in successful directions. Molecular simulations will be applied with the aim to predict the materials features and their performance in industrial processes.

Impacto:

This is a multidisciplinary research project that involves fields like chemistry, physics, engineering, biology, and medicine. The results will be of industrial and environmental interest. Among a number of examples, molecular modelling in porous materials can play a useful role in processes involving water, carbon dioxide capture, and methane storage.

Presupuesto: 1,369,080.00

Equipo de investigación

Nombre: Nanostructured materials for technological applications
Email: scalero@upo.es
PAIDI: FQM319
Web: http://www.upo.es/raspa/
Investigador principal: Sofía Calero Díaz (Principal Investigator)
Email: scalero@upo.es
Presupuesto del equipo: 1,369,080.00

Universidad: Universidad Pablo de Olavide

Enlace: http://www.upo.es/raspa/

Estado: published

Contacto **Solicitar más información de Towards more efficient materials for technological processes**