On the design of optimal porous crystals for adsorption and purification processes

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In September 2000, we launched the Materials Modelling and Simulation (MSM) Group at the Department of Applied Physics, Eindhoven University of Technology, the Netherlands. This group uses high-performance computers to simulate materials that can revolutionise renewable energy and green technology. The MSM group is integrated with the Eindhoven Institute for Renewable Energy (EIRES) and the Eindhoven Artificial Intelligence Systems Institute (EAISI). In this unique environment, and in close collaboration with industry, we develop and apply both quantum and classical methods, jointly encompassing a comprehensive multiscale approach to study complex materials and molecules from the atomistic to the nanoscale. The systems we are currently focusing on include, among others, porous crystalline materials, novel semiconductors and hybrid nanomaterials [1,3]. This invited lecture will focus on the former, discussing the state of the art, current work and what we foresee in the short and long term.

Crystalline porous materials have much to offer. However, establishing unique relationships between chemical composition, physical properties and their functionalities in the final application is still a chimera. Our motivation is to use theoretical analysis and computational modelling to "invent" materials and redesign processes that respond to the current energy and environmental challenges of our society . To this aim we use our own methodology, force fields and software [4-7]. The RASPA software is a classical general-purpose simulation package especially suited to study adsorption and diffusion in nanoporous systems. In addition, we have recently implemented iRASPA which is an advanced visualisation package. These software package are optimised to be fast and accurate, allowing a quick evaluation of the structures of storage and/or separation devices (ref RASPA and iRASPA).

For effective adsorption and separation, it is necessary to find materials with high adsorption selectivity and suitable capacity for use in the traditionally used fixed-bed devices . Therefore, crystalline structures need to be examined for their ability to perform gas separation based on adsorption equilibrium, selectivity, diffusion, permselectivity, structural characteristics and kinetics. In most cases, the efficiency depends mainly on the optimal combination of selectivity and effective pore volume, and this can be obtained from our simulations and experiments[8-10]. I will discuss all these issues, as well as the development of high-throughput methods to automatically calculate properties and provide adsorption processes. I will conclude by showing some innovative approaches to assess material stability and to identify and design high-performance, stable crystalline porous materials.

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