BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA

INSTITUTO DE FÍSICA
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SEMINARIO EXTRAORDINARIO
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"Quantum Effects on the Diffusivity of Hydrogen Isotopes in Zeolites"

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The molecular sieving of H_2 and its isotopes produced by nuclear plants is a long-standing research where some adsorption processes are well identified. However, some mechanisms governing the diffusion of the proton and its isotopes within a faujasite Na_X at low temperatures (40–100 K) are still troublesome to characterize. Notwithstanding, an understanding of the processes governing adsorption diffusion within narrow pores is essential for the development of recycling procedures of gases produced by nuclear plants. At cryogenic temperatures, it is well known that quantum effects are revealed and the heterogeneity of the guest structure plays an important role in the adsorption process. Here, we focus on the consequences of these two factors on molecular sieving and transport coefficients based on molecular dynamics including the Feynman–Hibbs quantum approximation. Our results show at temperatures below 77 K that H_2 has a lower adsorption capacity and a lower diffusion coefficient than those of D_2 and T_2. Here, we give an original explanation of this diffusion inversion in terms of the activation energies. We show that this energy is greater for H_2 by 30 and 50% than that for D_2 and T_2, respectively. Moreover, experimentally, it has been shown that the pore heterogeneity of the faujasite NaX leads to an increase of the self-diffusion coefficient with loading. For explaining this unexpected behavior, several authors have proposed a scenario based on either privileged adsorption sites or the residence time of molecules near the guest pore walls, followed by isotropic jumps. Here, we report an original analysis based on the mean square displacements, revealing the presence of slow and fast molecular mobility regimes. The ensemble of our results provide useful physical information about the development of recycling procedures of gases produced by nuclear plants.

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