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ABSTRACT:

Towards "infinite" selectivities in CO_2/CH_4 and CO_2/N_2 separations with MgNa-GIS flexible zeolite – A focus on adsorption

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Thanks to their perfectly tailored framework topologies, small-pore zeolites have received much attention in the last years for separation of small gases with high added values.[1]. However, finding the best zeolites for such task is not easy since many parameters have to be synergistically screened. In this context, we present a comprehensive study mixing DFT calculations and molecular dynamics simulations to isolate the best formulations for CO_2 separation. This first step led to the template-free synthesis of stable Na-GIS followed by partially ion-exchange with Mg^{2+} cations. The parent Na-GIS and partially-exchanged NaMg-GISs were thoroughly characterized using state-of-the-art techniques, and studied for their applicability for CO_2 adsorption and $CO_2/N_2/CH_4$ separation through single component adsorption at both low and high pressures and dynamic breakthrough curve analysis methods. In all cases, deep investigations were conducted using advanced and high-precision sorptiometry to understand the effect of the network dimensionality, flexibility and accessibility on the resulting adsorption behaviour and heat of adsorption values with pure component and gas mixtures. Finally, simplified fast cycling experiments consisting of five complete dynamic cycles were conducted to evaluate the potential of this material in pseudo realistic flow setups. Our findings revealed that NaMg-GIS zeolite exhibits highly promising potential for efficient CO_2 separation, outperforming the parent Na-GIS and reference zeolites in both CO_2/CH_4 and CO_2/N_2 binary systems. Of particular importance, NaMg-GIS demonstrated an "*infinite*" selectivity for CO_2 in the CO_2/CH_4 separation at both 25 and 50°C.

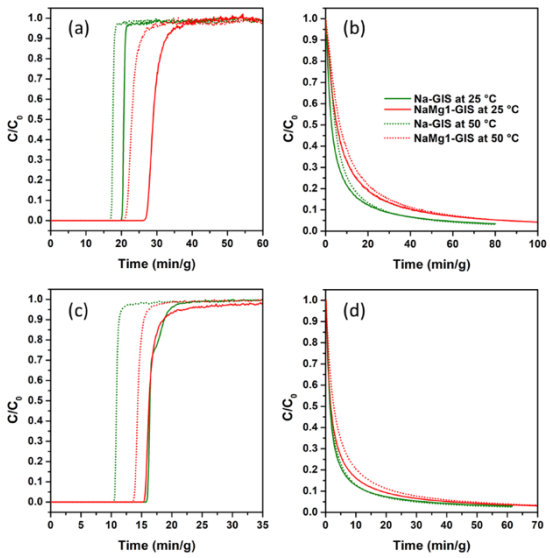

Fig. CO_2 breakthrough (a, c) and desorption curves (b, d) at 25 and 50 °C obtained from competitive dynamic adsorption experiments, CO_2/N_2/He, 5/25/70 (a,b) and CO_2/CH_4/He, 20/30/50 (c,d).

[1] M. Dusselier & M. E. Davis, Chemical Reviews 2018, 118 (11), 5265-5329.