Stepped Propane Adsorption in Pure-Silica ITW Zeolite

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Gas adsorption over zeolites is at the basis of important applications of this class of microporous crystalline solids, notably as separation media and catalysts, but it may also be complex and not straightforward to understand. We report that for temperature below 323 K propane adsorption on the small-pore pure-silica zeolite ITW exhibits a clear step (pseudosaturation). This is absent in the case of propene and the other small linear alkanes. An intermediate plateau, clearly observed in the 293 K isotherm, always occurs when one molecule of propane is loaded in every other cage, i.e., at half-saturation. The simulation results show a swelling of the ITW structure upon propane adsorption. The strong dependence of available pore volume on the adsorbate loading level implies that adsorption cannot occur on the void structure while saturation can only be reached on highly loaded structures. To account for this unprecedented adsorption phenomenon, we propose the term "guest-modulated effect".