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Gate Opening Transition of Zeolitic Imidazolate Framework – 8 in Xenon adsorption and Carbon Monoxide Adsorption. DINUKA H GALLABA, ALDO D MIGONE, Department of Physics, Southern Illinois University, Carbondale IL 62901, KARIM SAPAG, JHONNY VILLAROEL, Universidad Nacional de San Luis, San Luis 5700, Argentina. — Zeolitic Imidazolate Framework – 8 (ZIF-8) is a porous metal-organic framework material that shows flexibility in adsorbing larger molecules. We have investigated Xe adsorption on ZIF-8 for temperatures in the range between 95K and 157.5 K and we are exploring CO adsorption between 80K and 110K. ZIF-8 is known to undergo a structural (“gate-opening”) transition when sorbent loading increases. We report on this gate-opening phenomenon for Xe and CO on ZIF-8. The gate-opening transition appears as a sub-step at higher loadings in the adsorption isotherm data. For Xe the sub-step disappeared for temperatures above 145 K. All isotherms below this temperature clearly show the extra step. Gate-opening occurs as a result of the re-orientation of the organic linkers in ZIF-8. This re-orientation increases the size of the apertures in the structure, consequently allowing more molecules or atoms to adsorb into the ZIF -8 (which produces the additional sub-step). The isosteric heat of adsorption as a function of loading, and, the energy associated with the structural transition were determined from the adsorption data. We also report on the kinetics of sorption for Xe on ZIF-8: there are two rates that dominate the sorption kinetics on ZIF-8. We report on the values of the rates as a function of sorbent loading.

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