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Adsorption Selectivity between Hydrogen and Carbon Dioxide in Pelletized HKUST-1

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We aim to measure the adsorptive selectivity of HKUST-1 between hydrogen and carbon dioxide in the mixed-gas state by gravimetric gas uptake experiments performed at near ambient temperatures. The material of investigation, HKUST-1, is a metal-organic framework material of very high surface area (~ 1800 m²/g) and exceptional storage densities for gases which are of relevance for energy applications, especially H₂, CO₂, and CH₄. We specialize in the preparation of high quality samples of HKUST-1 in pelletized form, a consideration which has been very often overlooked in the previous literature but which is crucial for practical applications. The effects of pelletization on the pure gas adsorption uptake of HKUST-1 (and other MOFs) are not well known, and the effects on mixed-gas adsorption remain essentially unknown.

A complete study of adsorption selectivity between H₂/CO₂ requires of a number of individual isothermal adsorption measurements which we propose to carry out using a gravimetric magnetic suspension balance. The necessary set of pure gas experiments include: helium (to determine the skeletal density of the sample), hydrogen, and carbon dioxide. A number of gas mixtures should also be collected. Therefore, the required number of days is ~ 6 per working temperature of interest since each isotherm requires 1-2 days to complete. In addition, there should be enough time for sample pretreatment (activation): ~ 1 day. Therefore, the total number of days requested is ~ 20 . Analysis will then be performed by applying the IAST model to determine the equilibrium concentration of each gas species in the mixed adsorption state, from which the full complement of thermodynamic properties of this co-adsorption system can be ascertained.

We hope to be able to compare our results to the classic theory paper concerning adsorptive selectivity in HKUST-1: <http://pubs.acs.org/doi/full/10.1021/jp062723w>.