Hydrogen Adsorption and Its Displacement of Carbon Dioxide in Microporous Transition Metal Cyanides

SITTICHAI NATESAKHAWAT, JEFFREY CULP, CHRISTOPHER MATRANGA, BRADLEY BOCKRATH, U. S. Dept. of Energy, National Energy Technology Laboratory — The adsorption properties of H$_2$ and CO$_2$ have been investigated in M$_3$[Co(CN)$_6$] (M = Cu, Zn) Prussian blue analogues and M[Fe(CN)$_5$NO] (M= Co, Ni) metal nitroprussides. Adsorption isotherms show that both materials adsorb between 1.4 to 1.7 wt % of H$_2$ at 77 K and 1 atm. The isosteric heat of adsorption was between 6.5 to 7.5 kJ/mol. Kinetic measurements are conducted in a specially designed vacuum system which is coupled to a Fourier-Transform Infrared Spectrometer. In a typical experiment, an infrared active gas (i.e CO$_2$) is physisorbed in the transition metal cyanide and the system is later back-filled with H$_2$. The infrared intensity of the physisorbed CO$_2$ is monitored to deduce the kinetics and energetics associated with its displacement from the transition metal cyanide by H$_2$. We have identified several kinetic steps, measured the rate constants, and examined the temperature dependence of this displacement process.

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