Highly selective adsorption of CO over CO_2 and high CO/CO_2 selectivity by π-complexation using Cu(I) doped MIL-100(Fe)

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Octahedral metal-organic framework MIL-100(Fe) doped with Cu(I) for CO/CO2 separation were successfully synthesized by impregnation and consequent reduction under vacuum condition. Although MIL-100(Fe) adsorbs CO2 better than CO, Cu(I) doped MIL -100(Fe) shows selective CO adsorption over CO2 due to the π-complexation of CO and Cu(I). A series of systematic experiments on gas adsorption under the changes of metal loading, activation temperature, and adsorption temperature were thoroughly investigated. An optimized, CO adsorption capacity on Cu(I) doped MIL-100(Fe) was much higher than that of CO2. Single gas adsorption behaviors on MIL-100(Fe) and Cu(I) doped MIL-100(Fe) were well described by DSLF isotherms. IAS Theory (IAST) was applied to predict adsorption isotherms of CO and CO2 mixture and CO/CO2 selectivity as a function of bulk pressure. The obtained results showed that 45wt% Cu(I) doped MIL-100(Fe) had CO/CO2 selectivity of 420 at 298K and 1 bar, which was much higher than that of parent MIL-100(Fe) (0.10) at the same conditions.