INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: Development of Amine Functionalized Mesoporous Silica (KIT-6) for Carbon Dioxide Capture

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SHORT ABSTRACT

The doctoral work focuses on the development of amine functionalized mesoporous silica based CO_2 adsorbent. Mechanical, thermal, hydrothermal and hydrolytic stability of material are important parameters in designing an adsorbent. They decide the working limitation of the material during practical application. Additionally, physical properties such as specific surface area, pore volume, pore diameter and pore structure also affect the performance during application. In last few years, large varieties of mesoporous silica were discovered. Three dimensional mesoporous KIT-6with large interconnected pores is selected in this study based on its stability in extreme external conditions. KIT-6 shows the high mechanical stability (up to 4680 bar) and thermal stability (upto 900°C); possibly due to the presence of thicker pore wall and cubical structure. It also shows the stable structural properties even after ageing for six months in atmospheric conditions and one month in water at room temperature. In addition, after three days of ageing in boiling water, KIT-6 still retains its porosity. At high pressure, a good surface interaction is seen between KIT-6 and CO_2 without significant damage to the structure. KIT-6 also shows 2.38 wt% H_2 storage capacity at 30 bar and −196 °C. The highly stable KIT-6 is considered to be a good material for adsorbent, catalyst support and nanostructure synthesis. But low CO_2 sorption capacity at low partial pressure suggests further improvement in KIT-6 for practical application.

The CO_2 sorption capacity at low partial pressure is improved by grafting of APTES in highly stable mesoporous KIT-6. The grafting capacity of APTES on KIT-6 is tailored with increase in water

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concentration in the grafting solution (toluene). Presences of water in the grafting solution improves the APTES loading through double condensation. It shows an agglomeration of APTES and leading to a non-uniform distribution on KIT-6. However, the CO_2 sorption capacity is improved from 0.48 mmol/g (KIT-6) to 1.56 mmol/g (0.20KIT 9.0AP) at 1 bar and 30 °C.

The sorption capacity depends on the accessible amine group present for CO_2 in the adsorbent. The intensity of amine in the KIT-6 is further improved by grafting of TMPTA and compared the sorption performance with MCM-41 and SBA-15. It is found that the sorption capacity of KIT-6 is increased up to 2.59 mmol CO_2/g (WK30T) at 30°C and 1 bar. However, MCM-41 and SBA-15 show the maximum sorption capacity of 1.34 mmol CO_2/g (M20T) and 1.54 mmol CO_2/g (S20T), respectively at 30°C and 1 bar. After aqueous grafting of TMPTA, the sorption capacity of MCM-41 and SBA-15 are sharply decreased because of pore blocking and reduction in the accessible amine group.

CO_2 sorption capacity of aminosilane grafted KIT-6 gradually decreases with increase in adsorption temperature. Hereafter, CO_2 sorption capacity is further improved by impregnation of wide varieties of polyethyleneimines (DETA, TEPA, PEHA, PEI-800, PEI-1200 and PEI-25K) in KIT-6. The sorption capacity of polyethyleneimine impregnated KIT-6 is gradually increased with increase in temperature from 30 °C to 105 °C. In addition, KIT-6 shows better CO_2 adsorption performance than more traditional MCM-41, SBA-15 and HV MCM-41. The 60 wt% PEHA impregnated KIT-6 (K/60 PEHA) shows the maximum sorption capacity of 4.0 – 4.5 mmol CO_2/g at 90 −105 °C at 1 bar. The adsorbent is further improved by impregnation of polyethyleneimine in as-synthesized KIT-6 (ASK) in minimum time and energy. The confiscated structure directing agent within ASK improves the thermal stability as well as kinetics of adsorbent during CO_2 adsorption. The 60 wt% PEHA impregnated ASK shows the stable sorption capacity of 3.86 – 4.18 mmol CO_2/g at 90−105 °C and 1 bar. Thus, high sorption capacity at low partial pressure and high temperature illuminate ASK (particularly, 60wt% PEHA impregnated ASK) a promising candidate for CO_2 capture from large anthropogenic source.

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