Aligned Carbon Nanotubes as Porous Materials for Selective Carbon-Dioxide Adsorption and Desorption: Effect of Pressure and Charge

Principal Investigator
Dr. Jayant K. Singh,
Department of Chemical Engineering,
IIT Kanpur, Kanpur-208016
Email: jayantks@iitk.ac.in

Abstract:

The escalating level of atmospheric carbon dioxide is one of the major pressing needs for efficient deployment of carbon capture and storage at the major sources for reducing CO_2 emission. This is also regarded as a grand challenge of the 21st century. This projects aims to address carbon capture and storage aspects using novel techniques from a molecular perspective. The main goals of this research project is to gain a solid theoretical understanding of the adsorption/desorption behavior of CO_2 in presence of SO_2, NO_2 and H_2S and H_2O in 3D vertically aligned double-walled carbon nanotube (CNT) structures with charged/uncharged or/ and functional group (-NH_2) under low and high pressure (0 to 30 bar). CNTs are ideal porous model structures for otherwise unordered and less well defined carbon adsorbents. Such 3D CNT arrays with different sizes and spatial orientation of the arrays, variable intertube distances and CNT diameters, offer ideal model systems in which gas adsorption and desorption of environmentally critical gases can be studied by a combination of experimental and theoretical methods. Due to the defined CNT geometry on the nano, as well as on a micro and macroscale, the 3D aligned CNT structures are certainly of technological relevance. Due to their ideal 1D linear structure they are also valuable model systems, which allow to unravel underlying fundamental structure/property relationships of molecular interaction of these gases with the CNT inner and outer surface.