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A Molecular Dynamics Study on the Confinement of Carbon Dioxide Molecules in Carbon Nanotubes[1] MEAGAN LAZOR, DENIZ RENDE, NIHAT BAYSAL, RAHMI OZISIK, Rensselaer Polytechnic Institute — The influence of atmospheric carbon dioxide (CO_2) concentration on global warming is considered as one of the primary environmental issues of the past two decades. The main source of CO_2 emission is human activity, such as the use of fossil fuels in transportation and industrial plants. Following the release of Kyoto Protocol in 1997, effective ways of controlling CO_2 emissions received much attention. As a result, various materials such as activated carbon, zeolites, and carbon nanotubes (CNTs) were investigated for their CO_2 adsorbing properties. CNTs were reported to have CO_2 adsorption capability twice that of activated carbon, hence they received the most attention. In the current study, single walled carbon nanotubes (SWNTs) were used as one dimensional nanoporous materials and their CO_2 adsorption capacity was analyzed with Molecular Dynamics simulations. Results indicated that SWNTs are excellent CO_2 adsorbers and their effectiveness increase at low CO_2 concentrations. In addition, we showed that by varying temperature, CO_2 can be removed from the SWNTs, providing a simple method to reuse SWNTs.

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