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Capture and release of carbon dioxide by carbon nanotubes via temperature cycling[1] DENIZ RENDE[2], NIHAT BAYSAL[2], Yeditepe University, RAHMI OZISIK, Rensselaer Polytechnic Institute — Carbon nanotubes (CNTs) received remarkable attention since they were shown to possess many unique properties as well as being effective and stable adsorbent materials that make them potentially useful for gas storage and separation of various gas mixtures. In this study, the effect of temperature variations on carbon dioxide (CO_2) capture via single walled carbon nanotubes (SWNTs) and multi walled carbon nanotubes (MWNTs) were investigated with molecular dynamics simulations. SWNTs of type (10,10), (15,15), and (20,20) and MWNTs formed from the combination of these were simulated. The temperature was varied between 300 and 360 K. The results suggest that absorption of CO_2 into the CNTs were directly related to the internal volume of the nanotube, but the cross-sectional area of the tube entrance had a significant effect on the number of CO_2 molecules retained. The number of CO_2 molecules collected in CNTs gradually decreases with increasing temperature. Separate simulations were performed to understand the potential use of CNTs as thermal pumps to collect/discharge CO_2 molecules via temperature cycling.

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