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Molecular simulation of carbon monoxide gas adsorption on single wall carbon nanotubes for prevent of Greenhouse gas emissions by Aluminum and other industries

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Abstract: Monte Carlo simulations are used to model the probability of different outcomes in a process that cannot easily be predicted due to the intervention of random variables. It is a technique used to understand the impact of risk and uncertainty in prediction and forecasting models.Monte Carlo simulation can be used to tackle a range of problems in virtually every field such as finance, engineering, supply chain, and science.Monte Carlo simulation is also referred to as probability simulation. The Grand Canonical Monte Carlo simulations were performed to systematically study the adsorption and separation of noble gases on single wall carbon nanotube (SWCNT) bundles. Pure carbon monoxide gases, as well as , were simulated in carbon nanotube systems under various conditions. Adsorption data was collected at 273.15 K and 473.15 K over a wide range of pressures. Furthermore, the influence of pressure and temperature of the carbon monoxide on the adsorption behavior was investigated.result show that adsorption increase with high pressure and low temperature
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Keywords: “carbon monxide;adsorption gas”