ABSTRACT

The earth's average temperature is being elevated owing to burning of fossil fuels, explicitly releasing enormous amounts of Carbon (iv) Oxide (CO_2) into the atmosphere. Therefore, effective collection strategies are needed to minimize the concentration of CO_2. The current work presents use of molecular simulations to examine CO_2 adsorption on zeolites. The zeolites were imported one after the other into material studio program and their symmetry was modified to P1 since adding the guest molecules would destroy any symmetry that could be present. Adsorption isotherm was picked as the Task and Metropolis for the Method. Among the 218 zeolites, the Linde Type A zeolite (LTA) stands out as the best for CO_2 adsorption with a percentage weight of 69.88% at 298 K and 1000 kPa. This calculated value is in agreement with a recent experimental study that reported 63.65 % at 298 K and 0.1 MPa, indicating that this model could be reliable in predicting the CO_2 loading capacity. SBN zeolite had a percentage weight of 50.63%, making it the second best CO_2 adsorbent and in comparison to LTA, it has a significantly smaller accessible pore volume and volumetric surface area Cloverite(CLO) comes third in ranking with a percentage weight of 50.13%. RTH is in the fourth position with a percentage weight of 42.23%. The structural features of the zeolites were also calculated and their significance on CO_2 adsorption, evaluated using a machine learning algorithm. Gravimetric surface area (GSA) of the descriptors seemed to be the most significant structural feature that influence CO_2 adsorption. Hence, the feature engineering may expedite adsorption of CO_2. Quantum chemical calculations were further used to provide insights into the sorption mechanisms, whereby it is thermodynamically favorable for CO_2 to adsorb through carbon bonding as opposed to dissociative adsorption or hydrogen bonding. Finally, the effect of doping the zeolites with selected cations on the loading capacity was investigated, whereby doping LTA with lithium significantly improved the adsorption of CO_2.