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Water molecules adsorption by a porous carbon matrix in the presence of NaCl impurities using molecular dynamic simulation

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Abstract

Today, one of the most important issues in human societies is environmental protection and material recycling. Due to their high surface area and high porosity, porous carbon can be used in different fields of catalytic, recycling, separation, storage, drug delivery, etc. In the present study, the process of adsorption of H_2O molecules in the presence of NaCl impurities by a porous carbon matrix has been investigated using the molecular dynamics method. The results show that the process of adsorption of H_2O molecules by the porous carbon matrix decreases with increasing impurities in atomic structures. Increasing impurities in atomic structures disrupt the process of adsorption of H_2O molecules by the porous carbon matrix. Numerically, by increasing the impurity to 20%, 56% of the H_2O molecules were adsorbed on the simulated atomic matrix. Also, the increase in impurities in atomic structures increases the adsorption process of disturbing atoms by the porous carbon matrix. By increasing the impurity to 20%, 9% of the disturbing atoms were adsorbed on the simulated atomic matrix. Finally, by performing this simulation and investigating the effect of impurities on H_2O absorption by porous carbon structures, it is expected that an optimal process can be designed for water treatment, which is one of the most important challenges of human societies.