Ab initio molecular dynamics of the effect of aqueous carbon dioxide on the initial hydration of tricalcium silicate particle

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Recent innovations in the utilization of carbon dioxide (CO_2) in construction materials have contributed to the improvement of the mechanical properties of final products and the mineral sequestration of CO_2. Despite the increasing number of publications on this topic, there is still a lack of sufficient studies that explain the phenomena on a molecular scale. In this study, density functional theory (DFT) calculation of the interaction of CO_2 molecule and tricalcium silicate (Ca_3SiO_5) is employed for measuring the effect of different weight ratios of aqueous carbon dioxide molecules on the hydration of a particle covered with water molecules. The hydration process at the initial time is simulated using molecular dynamic (MD) calculation, and the mean squared displacements (MSD) of calcium ions in the tricalcium silicate particle are measured at 300 K temperature. The results show that the presence of the CO_2 molecules interacting with the water molecules reduces the adsorption energy; however, these values do not provide insight into later hydration times. The MSD of calcium ions in the system without CO_2 is lower compared to the system with addition of CO_2 . The consumption of water molecules and the formation of carbonic acid may hinder the participation of water molecules at the initial time step in the hydration process.