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H2O and CO2 confined in cement based materials: an ab initio molecular dynamics study with van der Waals interactions JAMES MORAES DE ALMEIDA, CAETANO RODRIGUES MIRANDA, Universidade Federal do ABC, ADALBERTO FAZZIO, Universidade de São Paulo — Although the cement has been widely used for a long time, very little is known regarding the atomistic mechanism behind its functionality. Particularly, the dynamics of molecular systems at confined nanoporous and water hydration is largely unknown. Here, we study the dynamical and structural properties of H_2O and CO_2 confined between Tobermorite 9Å(T9) surfaces with Car-Parrinello molecular dynamics with and without van der Waals (vdW) interactions, at room temperature. For H_2O confined, we have observed a broadening in the intra and intermolecular bond angle distribution. A shift from an ice-like to a liquid-like infrared spectrum with the inclusion of vdW interactions was observed. The bond distance for the confined CO_2 was increased, followed with the appearance of shorter (larger) intramolecular (intermolecular) angles. These structural modifications result in variations on the CO_2 symmetric stretching Raman active vibration modes. The diffusion coefficient obtained for both confined H_2O and CO_2 were found to be lower than their bulk counterparts. Interestingly, during the water dynamics, a proton exchange between H_2O and the T9 surface was observed. However, for confined CO_2, no chemical reactions or bond breaking were observed.

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