Molecular Dynamic Simulation for Studying Stability of Structure I CO_2 Clathrate-Hydrate

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Abstract

Environmentally, CO_2 removal in form of CO_2 hydrate in the ocean is one possibility of reducing the atmospheric concentrations of this greenhouse gas and assist in diminishing global warming. Considering the importance of CO_2 hydrates, this paper focuses on molecular dynamics (MD) simulations of structure I CO_2 hydrate. The goal is to study the stability of the clathrate at different temperatures. For achieving this purpose, energetic and structural properties are calculated. Equilibrium MD simulations are carried out to study the properties of fully occupied CO_2 clathrate-hydrate at 260, 270, 280, and 290 K using CVFF force field. A mixture of water and CO_2 placed in a cubic cell is used as a model system to simulate the CO_2 clathrate hydrate at 5 MPa during total simulation time of 200 ps. The cell parameters, stablization energies as well as radial distribution functions are computed. The obtained results at different temperatures indicate the hydrate stablility at low temperatures up to 280 K. Moreover, stablization energy outcomes reveals that CO_2 hydrate is more stable than the empty clathrate.

Keywords: Molecular dynamic simulation, CO_2 hydrate, Thermodynamic properties

Research Highlights

- CO_2 removal as a greenhouse gas in form of gas hydrates is studied in curent research.
- In order to study the structure I CO_2 hydrate MD simulations are developed.
- The static structure properties as well as energies, and thermodynamic properties are calculated.