Ab Initio Molecular Dynamics Study of Methane Hydrate Thermophysical Properties

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Ab Initio Molecular Dynamics (AIMD) simulations are performed for fully occupied methane hydrates. Methane hydrates are crystalline compounds which consist of cages of hydrogen-bonded water molecules that entrap methane at high pressures and/or low temperatures. They exist naturally near continental margins and in permafrosts and are believed to contain an energy content that is twice that of all other fossil fuels combined. Their thermophysical properties have been primarily determined experimentally although there is a lot of disparity among the results of different research groups. Nevertheless, these properties are essential for producing natural hydrates and performing risk assessment studies for the production process, so an ab initio method was used in this work in an attempt to provide more accurate results. The temperature range considered is 210K-323K which is suitable for energy-storing hydrates in natural settings. The second-order elastic constants, thermal expansion coefficient, and heat capacity are evaluated as functions of temperature. The elastic constants are used to follow the stability of the hydrate lattice at different temperatures, and the results are compared with experimental values. These results constitute the first ab initio set for methane hydrates and complement our previous work that established the elastic isotropy of these compounds and their ideal strength in different directions using Density Functional Theory.