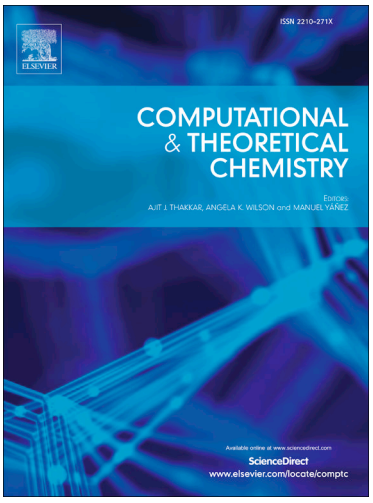

Dissociation mechanism of propane hydrate with methanol additive: a molecular dynamics simulation

Keyao Li, Ruili Shi, Yingying Huang, Lingli Tang, Xiaoxiao Cao, Yan Su, Jijun Zhao

PII: S2210-271X(17)30481-4
DOI: https://doi.org/10.1016/j.comptc.2017.11.011
Reference: COMPTC 2668

To appear in: *Computational & Theoretical Chemistry*

Received Date: 21 August 2017
Revised Date: 26 October 2017
Accepted Date: 8 November 2017

Please cite this article as: K. Li, R. Shi, Y. Huang, L. Tang, X. Cao, Y. Su, J. Zhao, Dissociation mechanism of propane hydrate with methanol additive: a molecular dynamics simulation, *Computational & Theoretical Chemistry* (2017), doi: https://doi.org/10.1016/j.comptc.2017.11.011

Dissociation mechanism of propane hydrate with methanol additive: a molecular dynamics simulation

Keyao Li[a], Ruili Shi[a], Yingying Huang[a], Lingli Tang[b], Xiaoxiao Cao[a], Yan Su[a*] & Jijun Zhao[a]

[a]*Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China*

[b] *School of Science, Dalian Nationalities University, Dalian 116600, P. R. China*

*** S Supporting Information**

Abstract: Employing NPT molecular dynamics method with consistent valence force field, dissociation processes of propane hydrate with and without methanol additive are simulated at different temperatures and a constant pressure of 50 MPa. We analyze structural snapshots, radial distribution functions, density distributions, angle distributions, change of energies, mean square displacements and diffusion coefficients of two comparative models and find that encaging methanol molecules in the 5^{12} cavities could enhance the diffusion behaviors of H_2O and C_3H_8 molecules and shorten the decomposition time of propane hydrate. The hydroxyl group of methanol could form hydrogen bonds with the water cage skeleton, and destroy the original hydrogen bond balance of the hydrate simultaneously. Our theoretical results could provide a useful guideline to understand gas hydrate blocking wellbore in the production and transportation of oil and gas.

Keywords: propane hydrate; decomposition; methanol; molecular dynamics