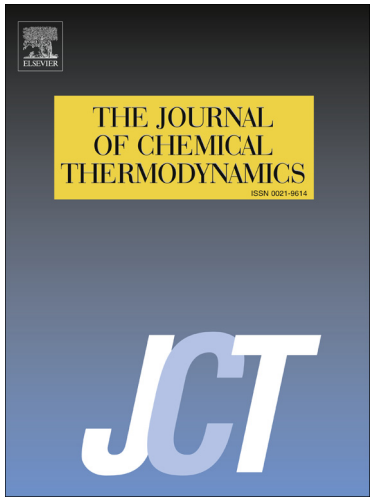

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Ab initio study of formation of the clathrate cage in the tetrahydrofuran hydrate

Jinxiang Liu[a,b], Shaofeng Shi[c], Zhenwei Zhang[c], Haiying Liu[b], Jiafang Xu[a], Gang Chen[b], Jian Hou[a*], Jun Zhang[d**]

[a]*State Key Laboratory of Heavy Oil Processing, College of Petroleum Engineering, China University of Petroleum, Qingdao, Shandong 266580, China*

[b]*School of Physics and Technology, University of Jinan, Jinan, 250022, China*

[c]*Linyi Academy of Technology Cooperation and Application, Linyi, 276037, P.R. China*

[d]*College of Science, China University of Petroleum, Qingdao, 266580, China*

Abstract: Despite the potential applications and ubiquity of clathrate hydrates, the molecular mechanism of formation of these compounds remains poorly understood. In the present work, we performed *ab initio* calculations to investigate the formation of the clathrate cage of the tetrahydrofuran (THF) hydrate and its significance to the adsorption of gas molecules such as the methane, carbon dioxide, and hydrogen. We found that THF and six water molecules cooperatively organize into an initial stable structure that will allow the growth of more water faces. The formation of the clathrate cage is thermodynamically feasible, and the water-THF interactions become more significant with the increasing water molecules. However, the water-water interactions mostly dominate the formation process due to the strong hydrogen bond interactions. Further, for the adsorption of the second guests, there is little change in the structure and stability of the clathrate cage, but these second guests favor to adsorb onto the pentagonal faces rather than the hexagonal faces.

Keywords: tetrahydrofuran hydrate; formation; adsorption; *ab initio* calculation

* Corresponding authors. Email: houjian@upc.edu.cn

** Corresponding authors. Email: sps_zhang@hotmail.com