Born-Oppenheimer molecular dynamics to the interaction of the methane hydrate with a vinyl caprolaptama polymer

A. C. Ramírez Gallardo,[1] G. Bravo-Pérez,[1] A. Romero-Martínez,[2] Humberto Saint-Martín[3] and I. García Cruz[1*]

[1] *Gerencia de Refinación. Dirección de Investigación en Transformación de Hidrocarburos, Instituto Mexicano del Petróleo, Eje Central Lázaro Cárdenas Norte 152, Col. San Bartolo Atepehuacan, C.P. 07730, Ciudad de México, MËXICO.*

[2] *Gerencia de Herramientas y Sistemas para Pozos e Instalaciones. Dirección de Investigación en Exploración y Producción, Instituto Mexicano del Petróleo, Eje Central Lázaro Cárdenas Norte 152 Col. San Bartolo Atepehuacan, C.P. 07730, Ciudad de México, MËXICO.*

[3]*Instituto de Ciencias Físicas, UNAM. Av. Universidad 2001, Cuernavaca, Morelos, 62210 MEXICO*

Abstract

In this work, we optimized the n = 15 clathrate interaction with the monomer and polymer of vinyl caprolaptama using Born-Oppenheimer molecular dynamics and a functional PBE+KS with dispersive (vdW) forces. The clathrate was previously obtained by Bravo and Saint-Martín[1] including dispersive effects and proved to be highly stable. In fact, this methane clathrate is the precursor of an n = 20 cage that lies 1.2 kcal/mol lower than the 5^{12} dodecahedral unit that takes part in crystal I.

It is already known the crucial importance of dispersive (vdW) forces in all this kind of intermolecular interactions.[2,3] We have considered three different orientations from the hydrate to monomer and polymer of vinyl caprolaptama, through different approaches, reaching in each case, 6-, 5-, and 4-ring faces of the clathrate. The results show that the methane hydrate in its interaction with the monomer and polymer of vinyl caprolaptama destabilizes mainly the water cage.

References

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