

***Ab Initio* Molecular Dynamics of Methane Hydrate Clathrates**

Fernando Alvarez Ramirez, Ascensión Romero Martínez and Isidoro García-Cruz^{C,S}
Instituto Mexicano del Petróleo, Programa de Ingeniería Molecular, Mexico City, México
igarcia@imp.mx

Methane hydrates denote different solid crystalline inclusion compounds in which, a hydrogen-bonded network of water molecules form fullerene-like polyhedral structures around trapped gas methane (or other simple molecules) allowing its stabilization. In this work, a theoretical study of the thermal effects on the electronic and structural properties of type II methane-hydrate clathrates is presented based on periodic boundary conditions models considering one methane molecule per cage. The thermal effects are inserted through *ab initio* molecular dynamics (*ab initio* MD) in a NVT ensemble with a simulation temperature of 270 K controlled by Nosé-Hoover thermostat. The pressure effects are analyzed carrying out different *ab initio* MD calculations, varying the cell length from 10.4 Å to 11.0 Å. The minimum energy crystal length was obtained at ~11 Å, which is smaller than the reported value of 15 Å which implies the presence of larger methane molecules inside the crystal cages. The thermal and cell length on the hydrogen bridge bond between the water molecules are analyzed through the mapping of the number of water molecules in the cell observing an increment of the water molecules when the cell length is close to 11.0 Å, which would be used to explain the transition from structure type I to type II of the hydrate formed. Finally, for all cases, it is observed a charge transfer, which is a function of the cell length, from the water clathrate to the methane along the *ab initio* MD.