CO clathrate hydrate stability with pressure : a DFT approach

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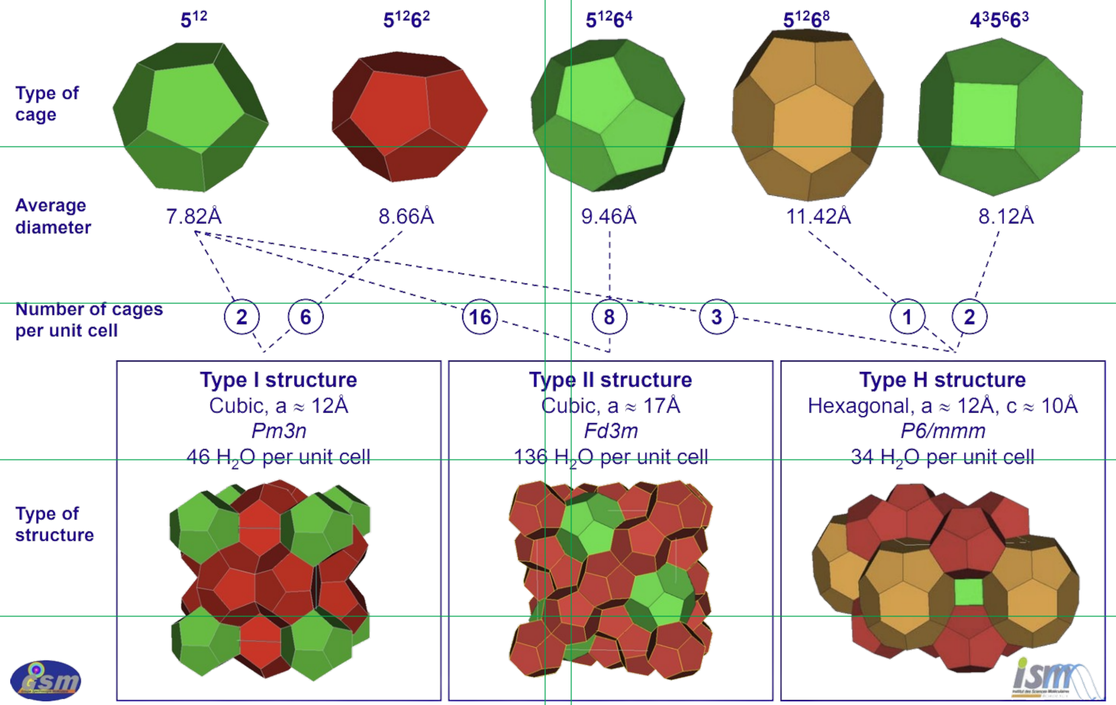
Abstract

After one hundred years to study the solid state of water, we still find another structure under specific conditions of pressure and temperature. One of the most interesting form is called clathrate hydrate, this state of ice can trap some or just one molecule of gas of different nature. Theses clathrathes hydrates can have many different structure and have different properties and have many application in industry. The CO-clathrate is an ice structure around carbon monoxide, in this lab work i have to study the stability with pressure for carbon monoxide for two different structures. In order to do that, i will use VASP a powerful software that perform quantum dynamics calculations based on the Density Functional theory called more commonly DFT.

Clathrhate hydrates

Clathrates hydrates can be stable with different structures their are for with 2-dimension planar elements, more precisely with tetrahedral network of water molecules and a guest molecules trap inside. They are different type of cage, the most important are : $5^{12}, 5^{12}6^2, 5^{12}6^4, 5^{12}6^8, 4^3 5^{16} 6^3$
They cage form unit cell and a type of structure with different average diameter respectively on their composition of type of cages.
The CO-clathrate is form with sI and sII structures :



references

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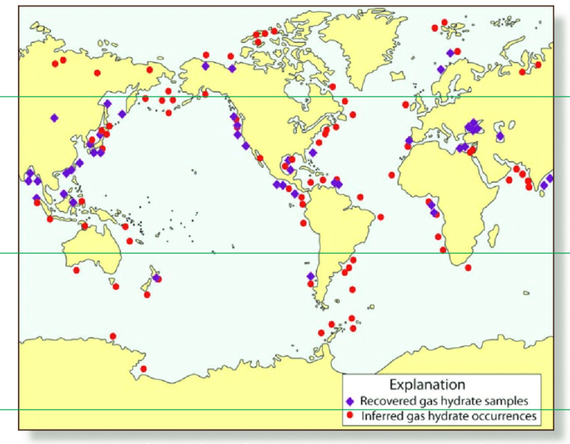
Application

On earth clathrate can be found in ocean and in permafrost because these environment have the necessary condition of temperature and pressure.
The discovery of clathrates hydrates was in 1810 when British scientist Sir Humphry Davy ,since this the industry was very interest by they application in many domain for example : in energy field because the most important clathrate on earth is methane hydrate (CH_4) and this is a huge quantity of potential energy, in pipeline for different reasons we have high pressure and high temperature and theses conditions favoring the formation of clathrate forming sealing in pipeline with a risk of explosion, theses structure can be a good solution to store gas.



Location of sampled and inferred gas hydrate occurrences worldwide. (Map courtesy of Timothy S. Collett, USGS)

Theory and future work

The stability and the dynamics of clathrates is perform with the Density Functional Theory, this theory can resolve the Schrödinger's equation to electronic structure for a atome or molecules. Unfortunately this equation has no analytical solution, the approximation of born Oppenheimer approximate the previous equation to :

$$H\Psi = \left[-\sum_i^N \frac{\hbar^2}{2m}\nabla_i^2 + -\sum_{i,I} \frac{Z_I e^2}{|\vec{r}_i - \vec{R}_I|} + \sum_{i<j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} + E_{II} \right] \Psi = E\Psi$$

The DFT solve this equation by considering electronic density functional and minimize it :

$$E[n(\vec{r})]\,(E[n(r)] = \langle \psi \,|\, T_e + V_{ee} + V_{ext} \,|\, \psi \rangle \rangle$$

2. Another sub section:

Subsection description