

CO clathrate hydrate stability with pressure : a DFT approach

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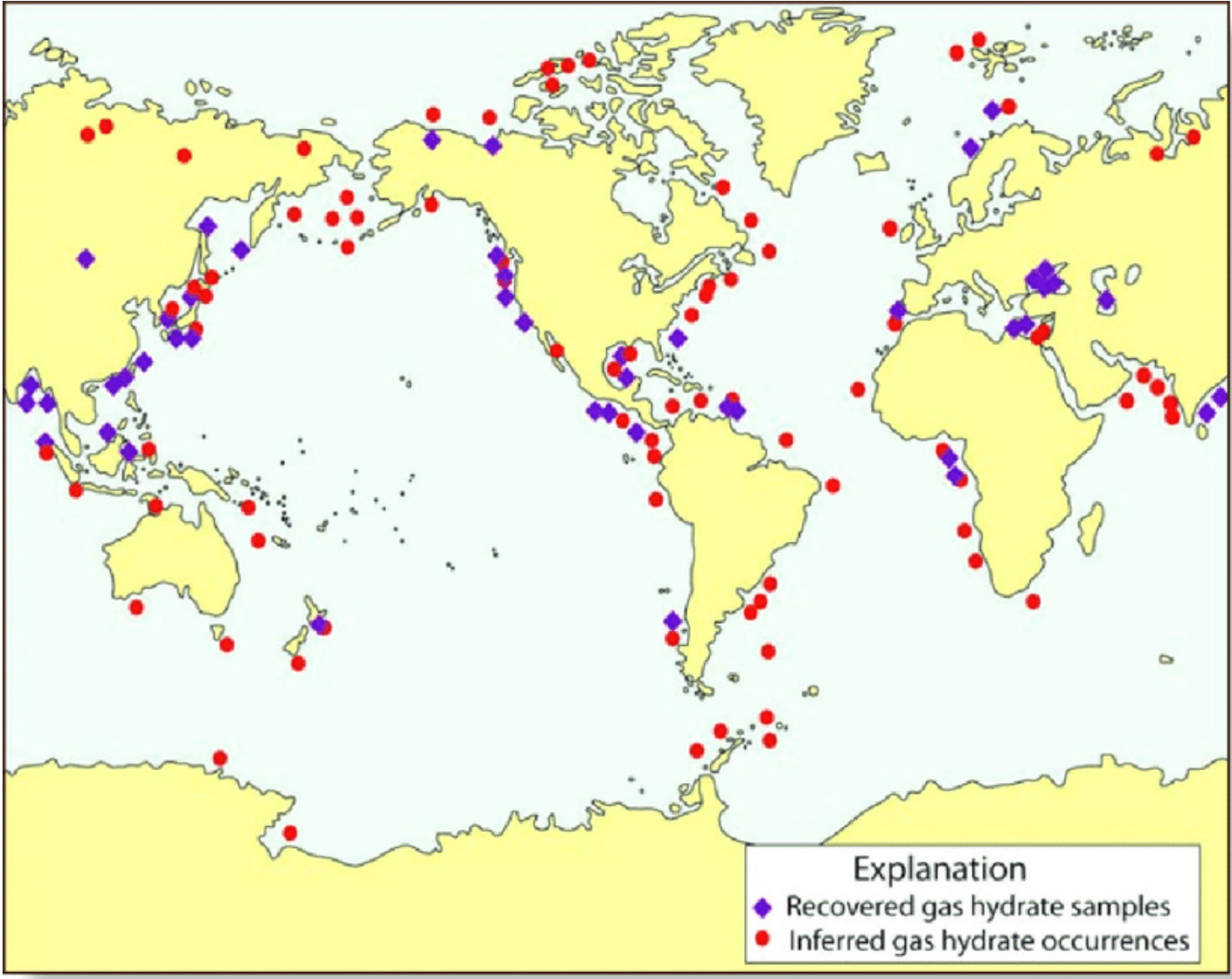


Abstract

Place an over view of your research - use your executive summary or abstract as a pointer of what information to place in here. 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 differ-ent structures their are for with 2-dimension planar elements, more precisely with tetra-hedral network of water molecules and a guest molecules trap inside. They are differ-ent type of cage, the most important are : $5^{12}, 5^{12}6^2, 5^{12}6^4, 5^{12}6^8, 4^35^{16}6^3$ 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 : qsdsgdqs On earth clathrate can be found in ocean and in permafrost because these environment have the necessary condition of temperature and pres-sure.



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

Theory

1. Introduction to sub section:

Subsection description



2. Another sub section:

Subsection description



3. Another sub section:

Final Subsection description



Application

The discovery of clathrates hydrates was in 1810 when British scientist Sir Humphry Davy ,since this the industry was very interest by they ap-plication in many domain for example : in en-ergy 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 favor-ing the formation of clathrate forming sealing in pipeline with a risk of explosion, theses structure can be a good solution to store gas.