הטכניון - מכון טכנולוגי לישראל

TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע"ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Special Seminar

Lecture Hall 6, Wolfson Department of Chemical Engineering,

Wednesday 15.3.2017 at 13:30

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Mechanisms of Gas Storage in Metal-Organic Frameworks

Hydrogen (H_2) and Natural gas (NG) are alternatives to gasoline as fuels for vehicles. However, despite having several advantages over gasoline, they both suffer from low volumetric density at ambient temperature and pressure such that storage of sufficient quantities requires specialized and bulky equipment for cooling or compression. Due to their high surface area and tunable properties, metal-organic frameworks (MOFs) are considered promising materials for gas storage applications. Ideally, gas can be stored by adsorption to the surface of the MOF where it takes up a much smaller volume compared to its standard state, enabling storage at lower pressures and higher density.

The challenge of designing materials with sufficient interaction with H_2 will be discussed in the first part of the seminar: It is commonly considered that coordinatively unsaturated ("open") metal-sites are required for significant H_2 attraction. This notion is challenged by studying several types of these sites and demonstrating that only metal-sites with specific arrangements of charges can exert sufficient polarization in the H_2 molecule and enable its storage. The adsorption of methane (CH_4) in MOF-5 is discussed in the second part of the seminar: By combining cluster-model DFT calculations with experimental data from CH_4 adsorption isotherms and neutron powder diffraction, we've identified the factors which control the adsorption process and determine the capacity of the MOF.

Refreshments will be served at 13:15