



THE CHINESE UNIVERSITY OF HONG KONG

Department of Physics

COLLOQUIUM

Hydrogen Adsorption Properties in Metal-organic Frameworks

by

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Time: 4:00 - 5:00 p.m.

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(Light refreshments will be served 20 minutes prior to the colloquium.)

ALL INTERESTED ARE WELCOME

Abstract

Due to the dwindling world-wide supply of petroleum along with environmental challenges due to CO₂ emissions, it is necessary to develop a sustainable and environmentally friendly energy system for transportation. One intriguing possibility is to use hydrogen as the energy carrier. Although substantial progress has been made over the past few years in developing fuel cells for transportation, there is still not a suitable hydrogen storage material. Recently, the synthesis of nano-porous materials with extremely large surface areas, including metal-organic frameworks (MOFs) and amorphous carbons, has led to some progress in understanding the adsorption of hydrogen molecules on material surfaces. However, there are still many technological obstacles to their future deployment. For example, the low H₂ adsorption enthalpy limits their application to low temperature; and the lack of understanding of surface packing density hinders the efficient improvement of H₂ uptake. To attack these problems, it is essential to have a detailed understanding of the physics of hydrogen adsorption properties in nano-porous materials. In this talk, I will present results on the hydrogen adsorption properties of MOFs with an eye to addressing these two issues. I will show that the hydrogen adsorption enthalpy can be greatly enhanced in many MOFs by exposing coordinatively unsaturated metal centers (CUMCs). Our results indicate that MOFs with exposed CUMCs generally show larger surface packing density at 77 K than those without CUMCs. In one special case, the hydrogen molecules on the surface can be packed even denser than solid hydrogen. We have also employed a simple model system to estimate the largest surface packing density for physisorbed hydrogen molecules on material surfaces. By using inelastic neutron scattering, the physical origin of this dihydrogen binding to CUMCs is also revealed.

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