Joint CQSE and CASTS Seminar

Weekly Seminar
Apr. 29, 2016 (Friday)

TIME Apr. 29, 2016, 14:30 ~ 15:30
TITLE Hydrogen storage properties of Li-adatoms adsorbed linear acenes studied by TAO-DFT with dispersion correction
SPEAKER Dr. Sonai Seenithurai
Department of Physics, National Taiwan University
PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Hydrogen adsorption in Li-adatoms adsorbed n-acenes (*m*Li-*n*Acene) has been studied by thermally assisted occupation density functional theory (TAO-DFT). When Li-adatoms are adsorbed on both sides of the hexagons of n-acenes, the adsorption binding energy of H_2 increases to the ideal binding energy range for ambient condition application. The first and second set of H_2 molecules adsorb on *m*Li-*n*Acene with the desirable binding energy range (20-40 kJ/mol/H_2). The hydrogen storage capacity of *m*Li-*n*Acene is 9.91–10.78 wt% which could be useful to design a storage medium that satisfy the USDOE's ultimate system target of 7.5 wt\%. Based on our results, *m*Li-*n*Acene are viable medium for hydrogen storage application at near ambient condition.