Joint CQSE and CASTS Seminar

Weekly Seminar
Dec. 11, 2015 (Friday)

TIME Dec. 11, 2015, 14:30 ~ 15:30
TITLE Determination of Adsorption Potential in Porous Materials Using Simulation Techniques
SPEAKER Prof. Bor Kae Chang
Department of Chemical and Materials Engineering,
National Central University
PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Simulations are a powerful set of tools for the modern scientist, especially with the rapid development of computers in the past decades and the accompanying increase in computing power. But what is modeling and simulation? How can we use these concepts to study real world engineering problems? This talk will endeavor to answer (or at least begin a conversation on) these questions starting with a small introduction on the technique called density functional theory (DFT), a type of "first principles" calculation. A demonstration of using this method to simulate a metal-organic framework (MOF) material shows how experiments that are impossible in the physical laboratory can be investigated computationally. A further example of gas adsorption in the MOF illustrates how computational and physical experiments can work together to allow scientists and engineers to form a more complete picture of the system of interest.