Séminaire de Chimie Théorique

Salle réunion groupe THEO 3ème Est, Bat. A12
Lundi 24 Septembre 2012 à 16:00h

Dr. Alejandra E. MARTINEZ

Grupo de Fisicoquimica en Interfases y Nanoaestructuras
Instituto de Fisica Rosario (CONICET-UNR)
Av. Pellegrini 250
2000 Rosario
ARGENTINA
mail: martinez@ifir-conicet.gov.ar
web: http://meteoro.fceia.unr.edu.ar/Gas-Surface/

H_2 dissociative adsorption on substitutional surface alloys

We will review recent theoretical work focused on H_2 reactive adsorption dynamics on substitutional surface alloys: Cu/W(100) and Pd/Cu(111). In both cases, the surface alloy electronic structure and the molecule-surface interaction potential is investigated through Density Functional Theory calculations. Reactive dissociative adsorption probabilities as a function of the molecular impact energy as well as the angular distribution of unreactive scattered molecules are analyzed and connected with the most relevant mechanisms observed: direct and dynamic trapping.

Contacts : p.larregaray@ism.u-bordeaux1.fr