Theoretical molecular dynamics with surfaces and PAHs

ARCHES* and IRSAMC† workshop

IRSAMC seminar room, Université Paul Sabatier, Toulouse, 26 may 2011

8h55	Opening		
9h	Bruno Lepetit	LCAR, Toulouse	Hydrogenation of graphene
9h30	Sabine Morisset	PIIM, Marseille	Sticking of a H atom on a graphite surface
10h	Rocco Martinazzo	University of Milan	Hydrogen formation on graphitic surfaces: energetics and dynamics of elementary processes
10h30	Coffee break		
11h	Geert-Jan Kroes	Leiden University	Achieving chemical accuracy for molecule-surface reactions
11h40	Cédric Crespos	ISM, Bordeaux	Theoretical investigation of the Eley-Rideal recombination of Nitrogen on Tungsten(100)
12h10	Mark Somers	Leiden University	Static surface temperature effects on the dissociation of H2 on Cu(111)
12h40	Lunch break		
14h30	Dominique Teillet-Billy	ISMO, Orsay	H atoms on graphenic surface: adsorption, abstraction
15h	Yves Ferro	PIIM, Marseille	Interaction of Be with graphite
15h30	Bret Jackson	UMASS, USA	Reaction Path approach to gas-surface reactive of Hydrogen-containing molecules
16h	Coffee break		
16h30	Sven Nave	ISMO, Orsay	Methane dissociation on Ni(111) and Pt(111): Energetic and dynamical studies
17h	Mathias Rapacioli	LCPQ, Toulouse	Modelling molecules and clusters with the Density Functional based Tight Binding method
17h30	Aude Simon	LCPQ, Toulouse	Atoms (Fe, Si), molecules (H2O) and clusters ((H2O)n) on the surface of a PAH: molecular dynamics simulations
18h	Discussion - End		

*GDR CNRS 2998 “Adsorption, Réactivité et Contrôle de l’ Hydrogène En interaction avec des Surfaces”, `http://www.u-cergy.fr/GDR-ARCHES`

†FR CNRS / UPS 2568 “Institut de Recherche sur les Systèmes Atomiques et Moléculaires Complexes”, `http://www.irsamc.ups-tlse.fr`