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***Rationalizing the $S(^1D) + H_2$ cold reaction dynamics
using a simple semi-classical statistical model***

In the last decade, quantum and semi-classical statistical models have proven fairly accurate at predicting reactive cross-sections as well as state/spatial distributions in the products of triatomic insertion processes such as the title reaction. The main advantages of such theoretical treatments are numerical simplicity and interpretative power. A simple semi-classical statistical model is presented here and its relevancy down to very low collision energies (5-120K) is evidenced for the $S(^1D) + H_2$ reaction by comparison with recent exact quantum scattering calculations [1-3] and molecular beams experiments [1-2].

[1]- Berteloite *et al.*, Phys. Rev. Lett. , 2010, 105, 203201

[2]- Lara *et al.*, Phys. Chem. Chem. Phys., 2011, 13, 8127

[3]- Lara *et al.*, Phys. Chem. Chem. Phys., 2011, 13, 8359

***Theoretical description of reaction dynamics:
from gas-phase to gas-surface elementary processes***

The goal of reaction dynamics is to understand the motion of atoms at the origin of elementary chemical reactions. To that end, state-resolved integral or differential cross-sections are usually measured in molecular beams experiments, revealing the state and/or spatial distributions of the products. From the theoretical point of view, quantum/classical molecular dynamics simulation and models help rationalizing the underlying physics. This is here illustrated with two examples concerning elementary processes in the gas phase and at the gas-solid interface.

We first focus on insertion atom-diatom reactions involving long-lived intermediate complexes. For processes of this kind, the dynamics might be accurately described using quantum and/or semi-classical statistical models. Here, a simple semi-classical capture model is presented, and applied to the $S(^1D) + H_2 \rightarrow SH(^2\Pi) + H$ reactive collision, leading to a nice agreement with recent exact quantum scattering calculations and molecular beams experiments.

The second part of the talk is devoted to diatomic recombination processes taking place at the gas-solid interface. The theoretical description of such mechanisms is of fundamental and practical in surface chemistry and physics. Using the Classical Trajectory method, the dynamics of molecular recombination of nitrogen (N_2) from a Tungsten (W/100) surface is investigated, focusing on the Eley - Rideal (ER) mechanism. The study relies on a recently developed potential energy surface based on an extended version of the periodic London-Eyring-Polanyi-Sato (LEPS) function. The influence of surface temperature on the reaction dynamics is approximately accounted for using the Generalized Langevin Oscillator (GLO) model.



Pascal Larregaray is a reasearch scientist at the CNRS (Centre National de la Recherche Scientifique, Bordeaux, Talence, France) specialized in theoretical chemical physics. He received a Ph.D. degree in chemical physics in 2001 from the Université Bordeaux 1 where he worked on Transition State Theory. In particular, he developed analytical models to account for post-transition state dynamics with a statistical approach. In 2002, he joined CERMM to work on simulations of collision induced dissociation of small metallic clusters in collaboration with Gilles Peslherbe. From 2003 to 2004, he undertook an assistant professor position at the EPFL (Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland) to investigate the medium local relaxation following a chromophore electronic excitation in supercritical fluids and quantum solids. In late 2004, he joined CNRS where he focuses on the theoretical treatment of gas-phase and heterogeneous elementary reaction dynamics..

