Seminář RCPTM – Dr. Didier Lemoine

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Název přednášky: Quantum studies of Ag(100) subsurface hydrogen atoms and of Eley-Rideal reactions between hydrogen atoms on Ag(111)

Abstract : In the ITER nuclear fusion reactor plasma heating will be mainly accomplished by the injection of highly energetic neutral atoms (D) obtained from a negative ion (NI) source. One innovative approach for the development of such a source is based on cold hydrogen plasma and involves two steps: i) efficient production of vibrationally-excited hydrogen molecules desorbing from a surface upon which hydrogen atoms stick and recombine; ii) followed by the process of dissociative attachment with the slow electrons of the plasma. The first step of this creation mechanism relies on weak atomic adsorption energy. Conversely, associative detachment with atomic hydrogen is an important loss mechanism of NIs in the plasma volume. Then, large atomic adsorption energy may minimize these losses. In close collaboration with experiments of S. Béchu *et al.* [AIP Conf. Proc. 1097 (2009) 74-83] we aim at characterizing surface materials that either trap and retain the atoms (minimization of volume losses) or generate efficiently molecules in a highly-excited vibrational state (which facilitates gains via dissociative electron attachment).

The adsorption of hydrogen atoms is weak on silver surfaces in comparison with most other metal surfaces and one may therefore expect a competition between the creation and loss mechanisms mentioned above. Another motivation for studying silver surfaces is to make up for the absence of theoretical modeling of the recent experiments of Kolovos-Vellianitis and Küppers [Surf. Sci. 548 (2004) 67-74]. They have characterized the thermal desorption spectroscopy (TDS) of H and D atoms from both Ag(100) and Ag(111), as well as the kinetics of the HD recombination reaction on both surfaces from the abstraction of D adsorbates by gaseous H atoms. Some of their results are quite unusual for metal surfaces. Notably, the TDS spectra evidence for Ag(100) a subsurface H or D population much exceeding that of the surface adsorbates with in addition, strong, intriguing isotopic effects. Also, the kinetics modeling gives rise to unprecedented, very large abstraction/recombination cross sections for Ag(111).

Density functional theory is used to generate the insertion and resurfacing paths of hydrogen atoms through Ag(100) as well as the potential energy surfaces for the Eley-Rideal recombination reaction on Ag(111). Quantum wave packet dynamics is performed to compute the Eley-Rideal reaction cross sections and vibrational distributions for three isotopic combinations involving H and D, over a thermal collision energy range encompassing that of the experiments. The results are compared with and/or complement those deduced from the experiments. They are also used to make predictions on the feasibility of a silver-based NI source.