UNIVERSITÀ DEGLI STUDI DI MILANO

# SEMINARI CHIMICI

Data

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Oratore

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Titolo

## Quantum studies of the interaction and reaction of hydrogen atoms with silver surfaces

Coordinatore

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In the ITER nuclear fusion reactor project plasma heating is mainly accomplished by the injection of highly energetic neutral atoms (D) obtained from a negative ion source. A promising approach for the development of such a negative ion 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 a weak adsorption energy of the atoms. Conversely, associative detachment with atomic hydrogen is an important loss mechanism of negative ions in the plasma volume. Then, a large adsorption energy of the atoms may minimize these losses.
In close collaboration with experiments in Grenoble, France [1] 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). It is also useful to determine optimal functioning conditions (plasma temperature, surface temperature, …). 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 Kuppers on the abstraction of D on Ag(100) and Ag(111) by gaseous H atoms [2]. To start with we generate the potential energy surfaces (PES) for the interaction of a single hydrogen atom through electronic structure calculations relying on density functional theory. They will be used to compute sticking properties that play a role in both the creation and loss mechanisms. The most favorable adsorption occurs above the hollow site. We also need to generate a PES for the Eley-Rideal recombination reaction. To this end we consider an incident H atom interacting with another H adsorbed above the hollow site.

[1] S. Bechu, D. Lemoine, M. Bacal, A. Bes and J. Pelletier, AIP Conf. Proc. **1097** (2009) 74-83
[2] D. Kolovos-Vellianitis and J. Kuppers, Surf. Sci. **548** (2004) 67