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ATTI DEL CONGRESSO

ORG/CTC-OR-04 L-Arabinose adsorption on a Ru cluster

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Use of bio-mass for energy, chemicals and material supply is one of the key issues of sustainable development, because bio-based resources are both CO_2-neutral and renewable, at variance with fossil fuels. Carbohydrates are the main source of renewables employed for the production of bio-based products. Therefore, chemistry know-how on industrial processes, involving carbohydrates is a subject of basis importance. Adsorption of the monosacharide L-Arabinose on a ruthenium nanocluster is here presented as an example of a catalytic system of potential industrial interest [1]. L-Arabinose can be found in aqueous solution in 5 tautomeric forms (*i.e.* α or β pyranose, α or β furanose and acyclic species) in equilibrium with each other. All these tautomers show a very large conformational flexibility, which previously has been also analyzed.

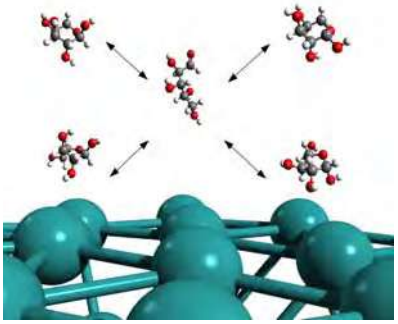

Figure 1. L-Arabinose on Ru surface

The L-Arabinose/Ru system has been investigated into the frame of the density functional theory (DFT). Calculations have been actually performed, using the DFT approach as implemented in SIESTA [2]. This employs linear combination of pseudoatomic orbitals as basis set. The atomic core is replaced by a non-local norm-conserving relativistic Troullier Martins pseudopotential, factorized in the Kleinmann-Bylander form.

The adsorption of different conformers, per each tautomers, on a Ru (0001) surface of the nanocluster have been modeled and analyzed in order to characterize the adsorption points both on the ruthenium surface and in the tautomeric species and to characterize if some of the latter are especially stabilized by the adsorption processes. Since adsorption phenomena could be affected by the adsorbate orientation, three different ways of binding per each conformers were investigated, considering either pyranose or furanose forms, and two for the acyclic forms.

[1] V. A. Sifontes, D. Rivero, J. P. Wärna, J. P. Mikkola, T. O. Salmi, *Top. Catal*., *53*, **2010** , 1278.
[2] J. Soler, E.Artacho, J. Gale, A. García, J. Junquera, P. Ordejón, D. Sánchez-Portal, *J.Phys.: Condens. Matter*, *14*, **2002** , 2745.