

#P173 - Plasma functionalization of gold nanoparticles for biosensing applications

Vittorio Ferrara - Dipartimento di Scienze Chimiche - Università degli Studi di Catania

Other Authors: Vittorio Ferrara (Department of Chemical Sciences, University of Catania, viale Andrea Doria 6, 95125 Catania, Italy), Patrizia Di Pietro (Department of Chemical Sciences, University of Catania, viale Andrea Doria 6, 95125 Catania, Italy), Cédric Vandennebeele (Chimie des Interactions Plasma Surface (ChIPS) Research Institute for Materials Science and Engineering Université de Mons (UMONS) & Materia Nova Research Center 1, Avenue Copernic, 7000 Mons, Belgium), Rony Snyders (Chimie des Interactions Plasma Surface (ChIPS) Research Institute for Materials Science and Engineering Université de Mons (UMONS) & Materia Nova Research Center 1, Avenue Copernic, 7000 Mons, Belgium), Cristina Satriano (Department of Chemical Sciences, University of Catania, viale Andrea Doria 6, 95125 Catania, Italy).

The present investigation deals with the functionalization of gold nanoparticles (Au NPs) with primary amine-based plasma polymer films (NH₂-PPF), to improve their properties for bioanalytical applications.

Cyclopropylamine (CPA) plasma polymerization, in pulsed and continuous wave radio frequency discharges, was employed to growth CPA amino-based PPFs coatings (18 nm) onto Au NPs of 12 nm of diameter deposited on glass and silicon substrates. A multi-technique investigation, based on FT-IR and XPS spectroscopies, AFM and SEM microscopies and ToF-SIMS spectrometry, revealed peculiar features of the CPA PPFs.

In particular, by FT-IR it was possible to obtain an overview about the rich chemistry of such PPFs, and by XPS, combined with chemical derivatization by using the reagent TFBA, it was possible to quantify unambiguously the surface -NH₂ amount. For testing the response in a biological environment, the behavior of the PPFs in phosphate buffer saline solution was studied upon 24 hours of immersion. The decrease of thickness occurred, related to a restructuring of the PPF structure induced by the diffusion of the solvent in the polymeric network. Such an effect of diffusion strongly depends on the cross-linking density of the PPF, characterized in the present study by ToF-SIMS. Despite such structural rearrangements, SEM does not show any evidence of delamination or damage caused after 24 hours of ageing in PBS. Results are therefore very promising for biosensor applications, as demonstrated by proof-of-work experiments with proteins and peptides.

#P174 - Palladium clusters on BNNT as catalysts for biomass conversion

Roberto Schimmenti - Dipartimento di Fisica e Chimica - Università degli Studi di Palermo

Other Authors: Remedios Cortese - Dipartimento di Fisica e Chimica, Università degli Studi di Palermo Antonio Prestianni - Dipartimento di Fisica e Chimica, Università degli Studi di Palermo Francesco Ferrante - Dipartimento di Fisica e Chimica, Università degli Studi di Palermo Dario Duca - Dipartimento di Fisica e Chimica, Università degli Studi di Palermo

The construction of a heterogeneous catalytic systems by a bottom-up approach is a fascinating strategy well assisted by molecular level characterizations. In this sense, DFT investigations can be used with predictive and descriptive purposes both for the treatment of the catalyst/support and for the substrate/catalyst characterization. This should be particularly useful for highly perspective but scarcely treated systems such as boron nitride based supports. Among these, boron nitride nanotubes (BNNT) have been demonstrated to have high chemical and thermal stability as well as great mechanical strength and high thermal conductivity.[1] Moreover, a high affinity toward hydrogen [2] as well as a moderate one to carbon dioxide, suggest their possible use as support for biomass conversion catalysts.

In this work we studied through computational methods, how small Pd₂ up to Pd₉ clusters can nucleate and grow on a BNNT support; the study of the interaction occurring between palladium clusters and the support can be highly revealing for the possible production of shape and size-controlled nanoparticles. We demonstrated that the migration process of a single palladium atom on the BNNT is not highly energy demanding and can be represented as a hopping mechanism between boron and nitrogen. A model was found for the interpretation of the growth energetics, showing that the process is generally favoured increasing the cluster size. Results from the adsorption of oxygenates compounds, as model for biomass feedstocks,[3] are discussed.

[1] M. Terrones, J. M. Romo-Herrera, E. Cruz-Silva, F. López-Urías, E. Muñoz-Sandoval, J. J. Velázquez-Salazar, H. Terrones, Y. Bando, D. Golberg, *Mater. Today*, 2007, 10, 30.

[2] M. Renzhi, B. Yoshio, Z. Hongwei, S. Tadao, Xu Cailu, Wu Dehai, *J. Am. Chem. Soc.*, 2002, 124, 7672

[3] R. R. Davda, J. W. Shabaker, G. W. Huber, R.D. Cortright, J. A. Dumesic, *Appl. Catal. B: Env.*, 2005, 56, 171

#P175 - Theoretical Investigation of Aqueous Phase Reforming of 1,2 Propanediol over a Pt catalyst

Roberto Schimmenti - Università degli Studi di Palermo

Other Authors: Remedios Cortese (Università degli Studi di Palermo), Francesco Ferrante (Università degli Studi di Palermo), Antonio Prestianni (Università degli Studi di Palermo), Dario Duca (Università degli Studi di Palermo)

Aqueous Phase Reforming (APR) process is one of the most efficient solution for producing hydrogen from biomass renewable feedstocks, such as polyalcohols. [1] Generally the reaction is catalyzed by supported platinum metals and among these platinum has been recognized as the most active and selective toward the production of hydrogen. However, due to its really high complexity, the reaction mechanism is today poorly understood.

DFT methods can be useful for understanding the APR catalytic mechanism at atomistic level. A detailed mechanistic study was carried out using a Pt₃₀ cluster for the modelization of the catalyst and 1,2 propanediol (1,2PDO) as a model feedstock for the APR. Even for this simple molecule five chemically different hydrogen atoms can be recognized which lead to five different reaction