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Veton HAZIRI

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The interaction of oxygen molecule at the Au(111)-Phenyl and Au(111)-Carboxyphenyl nano-layer interface. An experimental and Ab Initio study

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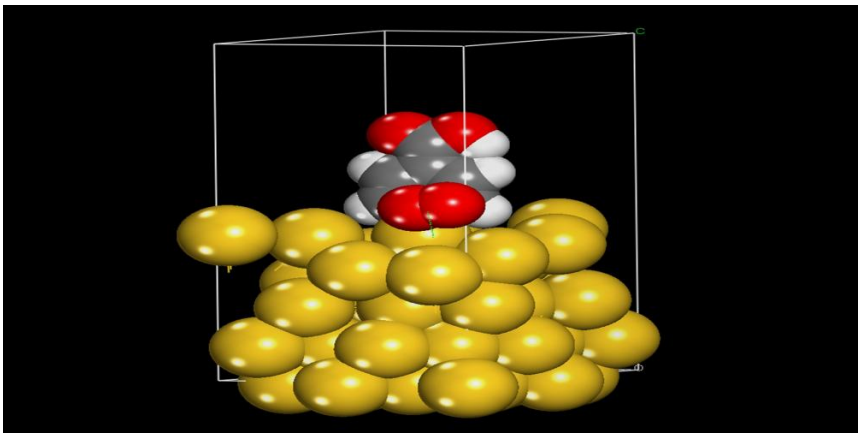

Surface modification via the aryl radicals derived from the de-diazotization reaction of aryldiazonium salts permits an elegant way to modify/functionalize different surfaces. In contrast to other methods (thiols, phosphonic acids, etc) it remains as the most efficient surface modification method regardless of the surface type (metal, semiconductors or insulator) that it can be applied. Although the structure of the modified surfaces by aryl layers is up to now well characterized experimentally by a number of different methods (XPS, Raman, IRRAS, AFM), the interaction of molecules such as oxygen with the formed interface remains up to now unknown. To elucidate how the oxygen molecule interacts onto the Au(111) modified surfaces by aryl groups (phenyl or carboxyphenyl), DFT calculations using Generalized Gradient Approximation (GGA) / DND basis set were performed for Au (111) surface modeled using a 4-layer model (under Periodic Boundary Conditions; cell dimensions: 9.99 Å * 9.99 Å * 7.951 Å with the addition of a 15 Å vacuum layer at the C axis) grafted by phenyl or carboxyphenyl groups. The interaction of the oxygen molecules (in the vacuum and water ? using Conductor like Screening Model) onto the bare and grafted gold surface was evaluated at different positions. The results gave important molecular insights regarding the adsorption energy and geometry induced changes upon the interaction of oxygen molecule onto the grafted interface.

Keywords: Oxygen Molecule, Au(111)-Phenyl, Au(111)-Carboxyphenyl, DfT, Cosmo

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SECM study of the formed oxygen bubbles onto Au(111)-Ph interface

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The study of the water/gas bubble interface is essential to understand the interaction of oxygen bubbles produced at working electrode. The formed gas bubbles as observed to migrate against the direction of the electrical field, an indication of their negative charge caused by the hydroxide layer at the bubble/water interface. In this study, the Au surface is grafted by hydrophobic nano-layer (derived from benzenediazonium). Oxygen molecules were generated by applying a positive potential on the tip of the working electrode (a platinum electrode). Afterwards, the SECM tip is approached toward the grafted substrate [Au(111)-phenyl] and the oxygen bubble was squeezed onto the top of the layer and then EIS measurements were obtained. An electrochemical system (EIS) can be modeled by an equivalent circuit. EIS data was analyzed using a Matlab code developed in our group. Electrochemical impedance spectroscopy measurements were achieved by applying an alternating current of 50 mV at 51 frequencies. EIS gave important results regarding the electrochemical behavior of the system.

Keywords: Oxygen bubble, Grafted Interface, Au(111), electrochemical impedance spectroscopy, Hydrophobic Layer,