Density Functional Theory study of Au-Cu alloy surfaces in presence of adsorbed gas: CO, NO and O_2

Marwa DHIFALLAH[a,b], Adnene DHOUIB[c], Sarah ALDULAIJAN[c]

Francesco DIRENZO[a], Hazar GUESMI[a]

[a] *Institut Charles Gerardt Montpellier, CNRS/ENSCM, 8 Rue de l'Ecole Normale, 34296 Montpellier, France*

[b] *Université de Gabes, Unité de recherche environnement, Catalyse et Analyse des Procédés, 6072 Gabes, Tunisie*

[c] *College of Sciences, Departement of Chemistry, University of Dammam, Dammam City, Saudia Arabia.*

In bimetallics the surface composition can be strongly altered by adsorbing molecules, the element with highest heat of adsorption segregating in the surface. To investigate the effect of reactive gas on the surface composition of Au−Cu alloy we examined by mean of Density Functional Theory (DFT) study the segregation behavior of copper in gold matrices. The adsorption mechanisms of CO, NO and O_2 gas molecules on gold, copper and gold-copper low index (111), (100) and (110) surfaces were analyzed from energetic and electronic points of view [1]. Our results show a strong segregation of Cu toward the (110) surface in presence of all adsorbed molecules. Interestingly, the Cu segregation toward the (111) and (100) surface could occur only in presence of CO and in a lower manner in presence of NO. The electronic structure analysis highlights the different binding characters of adsorbates inducing the Cu segregation.

References:

[1] M. Dhifallah, A. Dhouib, S. Aldulaijan, F. Direnzo and H. Guesmi,J. Phys. Chem. (2016) soumis