CO Adsorption-Induced Surface Segregation and Formation of Pd Chains on AuPd(001) Alloy.

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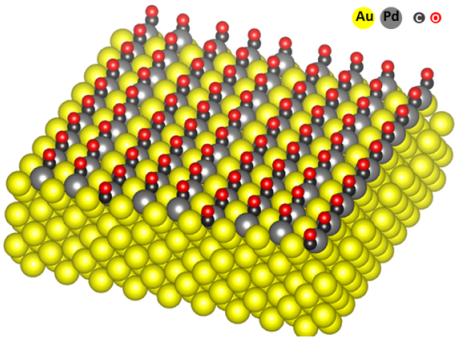

CO adsorption-induced Pd chains on AuPd(001).

In order to study how adsorption of CO molecules changes the surface composition of AuPd alloys, we develop a theoretical methodology which is able to take this effect into account. An Ising model based on DFT calculations is derived to define interatomic potentials that describe metal-metal, metal-CO and CO-CO interactions. Then, through the use of Monte Carlo simulations within the semi-Grand Canonical ensemble, the effect of adsorption-induced segregation on AuPd (001) surface is well reproduced for different temperatures and CO pressures : while Au segregates at the surface in Ultra High Vacuum conditions, a reversed Pd segregation is observed in presence of CO molecules [1, 2, 3]. Actually, segregation isotherms identify a Pd surface enrichment for low CO pressures and CO surface saturation is reached at an intermediate coverage of $\theta = 0.5$ ML. Furthermore, Pd chains induced by an ordering of the adsorbed CO molecules appear at low temperature and intermediate CO pressures. These chains are the result of a competitive effect between CO-CO repulsions and metal-CO interactions. Finally, we present a sketch of the phase diagram of the CO adsorption-induced ordered phase as a function of temperature and CO pressure.

1. Gao, F, Wang, Y, Goodman, D.W *CO Oxidation over AuPd(100) from Ultrahigh Vacuum to Near-Atmospheric Pressures : CO Adsorption-Induced Surface Segregation and Reaction Kinetics*, J. Phys. Chem. C 113, 14993-15000, 2009

2. Guesmi, H *Theoretical Insights on the Effect of Reactive Gas on the Chemical Ordering of Gold-Based Alloys*, Gold Bullet. 46, 213-220, 2013

3. Zhu, B, Creuze J, Mottet, C, Legrand B, Guesmi, H *CO Adsorption-Induced Surface Segregation and Formation of Pd Chains on AuPd(100) Alloy : Density Functional Theory Based Ising Model and Monte Carlo Simulations*, J. Phys. Chem. C 120, 350-359, 2016