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

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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 molecules¹,²,³. 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.