Comparaison between Pd-Au and Co-Pt surfaces segregation : a driving forces analysis

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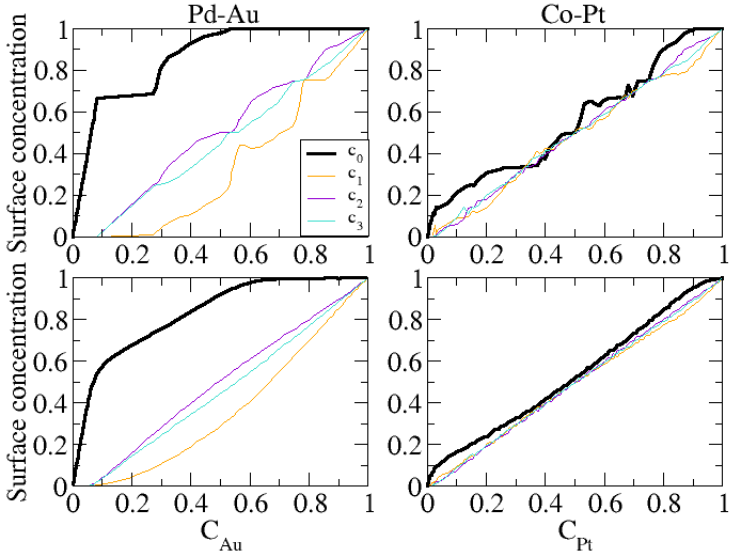
Pd-Au and Co-Pt alloys surfaces are very efficient for various catalytic reactions, in particular in the CO oxydation but also in the selective hydrogenation of 1,3-butadiene for Pd-Au system [1]. Surface ordering is the key to understand why these systems are so useful for catalysis. Experimentally, Gauthier *et al.* [2] showed that on Co-Pt(111), the probability to find CO on top of a Pt atom increases with the number of its Co nearest neighbors. Here we propose a theoretical study of surface segregation and surface ordering using Monte Carlo simulations and driving forces analysis.



(111) Surface concentration (surface c_0 and planes below c_1 , c_2 and c_3) as a fonction of Slab concentration C_{Au} (left) and C_{Pt} (right). At the top low temperature : 100 K for Pd-Au and 300 K for Co-Pt, at the bottom high temperature : 400 K for Au-Pd and 800 K for Co-Pt.

We performed it in semi-grand canonical ensemble with many-body potential which allows atomic relaxations. This potential has been fitted to ab initio calculations within the density functional theory.

Au-Pd is an ordered system which presents surprisingly a miscibility gap in the Au-rich side whereas Co-Pt is a typical ordered system. On the figure, we can see the effect on (111) surface segregation : a strong Au segregation for Pd-Au(111) surface and a slight Pt segregation for Co-Pt(111) surface. To understand the differences between the two systems we will analyse the segregation driving forces in terms of cohesive, alloying and size effect [3] derived within the semi empirical potential as it has been done before from DFT calculations for Pd-Au surfaces [4].

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