Supplementary information

Structural surface and thermodynamics analysis of nanoparticles with defects

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Pairwise interactions model versus EAM

Panel a) of the figure S1, shows the adsorption isotherm for an ICO NP whose seed is Au and the adsorbate is Ag. For the interaction potential, it has been considered the Embedded Atom model (EAM). EAM is well known for reproducing the main characteristics of metallic bonds, and consider many-body interactions in a functional way. The total energy of the system is obtained considering the sum of an attractive embedded energy contribution and a repulsive contribution from the interaction between ionic nuclei. The EAM contains parameters obtained from experimental data. This potential is described in detail in [1-3].The isotherm shown (panel a) was obtained with the MC simulation technique described in the manuscript. Panel b) shows the isotherm for the Hamiltonian with pairwise interactions (used in this work) for the same NP. For the former case, Ag-Ag and Ag-Au interactions are equivalent to w_{BB} and w_{AB}, respectively. As observed, both curves (a and b) present similar characteristics, i.e., two occupation plateaus formed by a big and a small occupation jumps (in that order going from more negative chemical potentials to more positive ones), until the maximum value is reached. The only difference observed is a shift of the chemical potential window where the total adsorption process occurs. From a computational point of view, EAM has a higher computational cost than that of the present work, however same results are observed in both cases

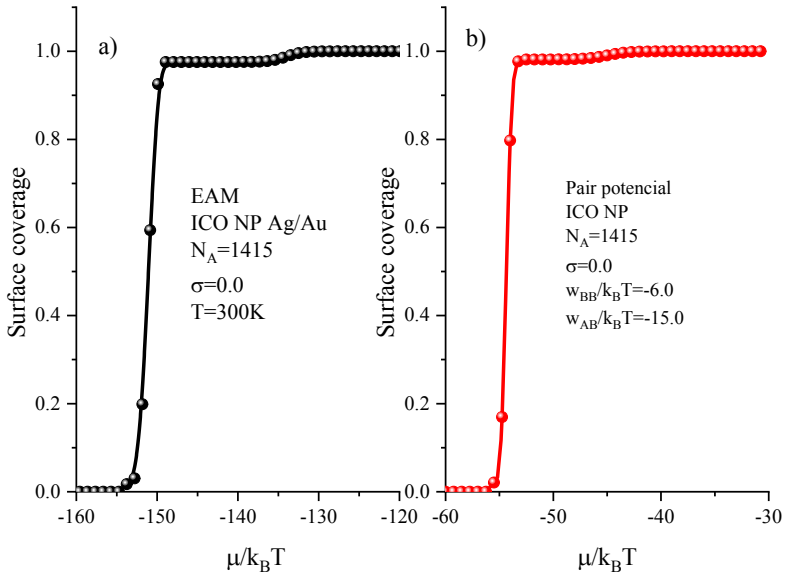

Figure S1: Adsorption isotherms for a clean ICO NP simulated with EAM Panel (a) and pairwise model (b)

References

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3) J.H. Li, X.D. Dai, S.H. Liang, K.P. Tai, Y. Kong,. , and B.X. Liu, Phys. Rep, 2008, 455 (1-3), 1-134