Surface structure and morphology of bimetallic alloys and nanoalloys: insights from numerical simulations

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The nanoscale structure of binary alloys is a key parameter that can be used to tune their properties for applicative purposes, such as for instance in catalysis, to improve reaction rates and selectivity. A representative case is the Ni-Cu system: its surface, whose local composition is crucially determined by segregation thermodynamics and kinetics, exhibits properties that are different from those of the constituent metals and from a simple linear interpolation (Figure) [1].

Nanoparticles, with low-coordination sites and finite-size effects, show different and often more convenient properties than single-crystal surfaces [2]. A further degree of freedom is offered alloying at the nanoscale. Alloy-based nanoparticles, or nanoalloys, show a fascinating variety of composition- and size-dependent structures and morphologies [3].

Numerical simulations based on complementary and different approaches, from quantum-mechanical to semiempirical potentials, combined with surface science experiments, allows to enter into the richness of structures and properties at the atomic-scale.

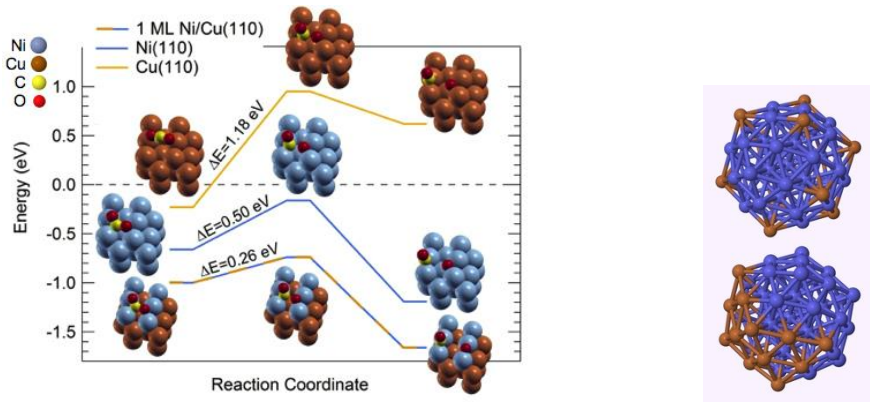

Figure caption: Left: Calculated energy diagram of CO_2 dissociation on the (110) surface of a bimetallic NiCu alloy and of the corresponding pure metals [2]. Right: Two different homotopes of a $Cu_{12}Ni_{43}$ icosahedral nanoparticle.

References:

[1] E. Vesselli et al., ACS Catal. **3**, 1555 (2013)

[2] Olmos-Asar et al., ACS Catalysis **5**(5), 2719 (2015)

[3] Panizon et al., Phys Chem Chem Phys (2015)