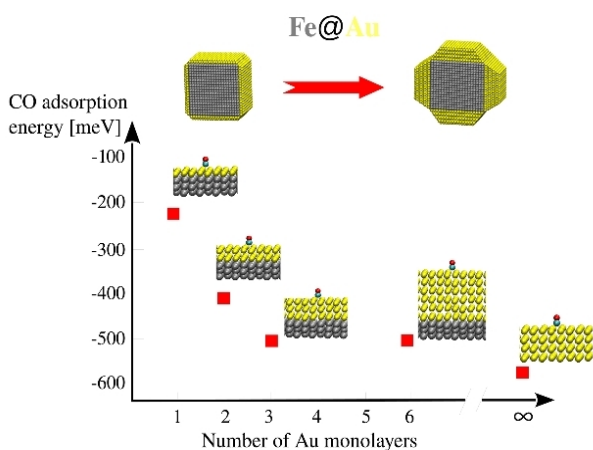


Adsorption energy of small molecules on core-shell Fe@Au nanoparticles : tuning by shell thickness

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Controlling the surface properties of metallic nanoparticles (NP) is one of the current major challenges since these properties determine the way the NPs interact with their environment - a crucial issue for catalysis and biomedical applications. One possible way to achieve a control of the adsorption of molecules on the surface of a NP is to control its morphology.



In this work, we show that it is possible to tune the adsorption energies of small molecules on the surface of core-shell Fe@Au NPs by using both strain and ligand effects. For this, we rely on the properties of faceted core-shell nanoparticles, in which the shell metal component is epitaxied on the core metal component. The lattice mismatch between the core and the shell causes the deformation of the shell surface and thus a change of its properties. Moreover, by varying the shell thickness, we show that additional change of the adsorption energies can be obtained using the ligand effect.

DFT calculations have been carried out on several molecules adsorbed on models of the core-shell Fe@Au nanoparticles obtained by vapor phase deposition¹. In particular, these NPs display Au(001) planes epitaxied on Fe(001) planes with the following orientation relationship Au(100) [011]//Fe(100)[010]^{2,3}. For carbon monoxide CO, the structural and energetic variations with the number of Au monolayers deposited on Fe have been analyzed and correlated with the distance between the carbon atom and the gold surface. The effect of the subsurface layer has been evidenced for 1 and 2 monolayers. The other molecules show different quantitative behavior depending on the type of their interaction with the gold surface. However, the iron substrate always weakens the interaction, either for the chemisorbed species or for the physisorbed ones.

1. C. Langlois, P. Benzo, R. Arenal, M. Benoit, J. Nicolai, N. Combe, A. Ponchet, and M. J. Casanove, *Nanoletters* **15**, 5075 (2015).

2. M. Benoit, C. Langlois, N. Combe, H. Tang and M.-J. Casanove, *Phys. Rev. B* **86**, 075460 (2012). and *Phys. Rev. B* **87**, 119905 (2013).

3. M. Benoit, N. Combe, A. Ponchet, J. Morillo, and M.-J. Casanove, *Phys. Rev. B* **90**, 165437 (2014).