Accurate surface and absorption energies from many-body perturbation theory

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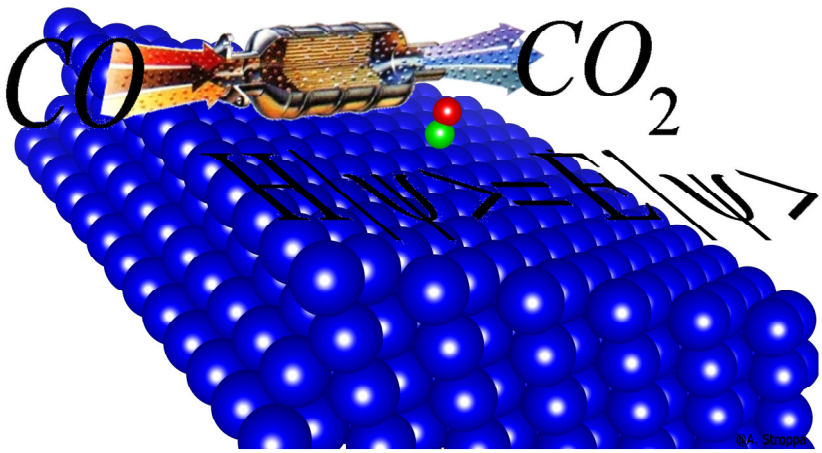
The exhaust gases produced by combustion engines of modern vehicles contain carbon monoxide (CO), a very toxic gas. The catalytic converters exploit the interaction of the CO molecule with metal surfaces, e.g. Platinum, in order to convert CO in CO2, a less harmful gas. The first step of the chemical reaction is the adsorption of CO on the surface. Despite its conceptual simplicity, the quantum mechanical modeling of CO adsorption based on density functional theory (DFT), the workhorse computational method in materials and surface science, poses serious problems. In the literature, this fundamental weakness is described as "CO adsorption puzzle". In 2008, A. Stroppa and G. Kresse (University of Vienna) have shown that using traditional local approximations to the many-body quantum mechanical problem either the stability of the surface or the interaction with adsorbed molecules is overestimated.
This was the 'smoking-gun' evidence that some piece of important physics was missing in traditional approaches preventing reliable computational catalysis modeling. In 2010, a joint collaboration between the University of Vienna and the CNR-SPIN Institute in L'Aquila, solved the "CO puzzle" by introducing a new way to calculate accurately the interactions in a many-electron system, namely the so called random-phase approximation. It enables us to calculate reliably all the properties of the reaction between molecule and metal surface including weak bonding effects due to van der Waals interactions. It is now possible to simulate complex catalytic process much more accurately making possible to design new materials for heterogeneous catalysis, pharmaceutical operations, hydrogen storage, materials development and alternative energy.



"Pictorial representation of the catalytic converter, CO adsorption on metal surface and quantum mechanical modelling"