**Theoretical investigation for Fischer-Tropsch reaction with metal nanoparticles: building a relevant structural model, a mandatory prerequisite**

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**Abstract**
The Fischer-Tropsch synthesis is a widely known catalytic reaction that converts carbon monoxide and hydrogen into liquid hydrocarbons: $(2n+1)\mathrm{H_2} + n\mathrm{CO} \longrightarrow \mathrm{C}_n\mathrm{H}_{2n+2} + n\mathrm{H_2O}$
Usually achieved within heterogeneous catalysis [1], nanocatalysts have also proven to be of interest as their special structural and electronic properties enhance their catalytic activity for Fischer-Tropsch synthesis as well as for a large range of reactions [2]. From the theoretical point of view, the study of such reactions implies the understanding of the nanocatalyst surface steric and electronic effects in order to be able to design relevant models usable as starting point for reactivity studies. We propose several tools in order to achieve such design: (i) molecular builder aiming at providing a wide variety of the typical shapes exhibited by nanoparticles, completed by the steric-driven grafting of ligands on its surface; (ii) reverse Monte-Carlo modeling, a general method that provides atomic structures based on experimental X-Ray or neutron diffraction data; (iii) *ab initio* thermodynamics [3], with the example of the adsorption and co-adsorption of dihydrogen and CO on ruthenium nanoparticles. *Ab initio* thermodynamics applied to hydrogenated ruthenium surfaces show a maximum coverage of 1H/ $Ru_{surface}$[4]. The same methodology applied to hydrogenated ruthenium nanoparticles evidence a larger saturation coverage (see figure below), in agreement with experimental observations [5]. Calculations on nanoparticles with coadsorbed CO and H give insight on the H/CO coverage under experimental conditions and therefore allows to perform reactivity studies on realistic models of nanocatalysts. This computational strategy examplified in the case of ruthenium nanoparticles for the Fischer-Tropsch reaction can be applied to any metallic nanoparticle.

**References**
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**Figures**