

# Theoretical interpretations towards catalytic experimental results

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Computational studies deal with modeling of some systems of interest in catalysis with the aim of explaining and interpreting experimental results. In the *first case* calculations were performed to elucidate the early stages of carbon rings with grapheme-like structures nucleation and growth on Pd(111), Ni(111) and Pt(111). In the *second one* the adsorption of CH<sub>3</sub>, CH<sub>2</sub>, CH, CH<sub>2</sub>OH, CH<sub>3</sub>O, CH<sub>2</sub>O and CHO species on a nanoparticle Pd<sub>79</sub> that mimics experimentally investigated model Pd catalysts. The structural, energetic and vibrational parameters of these adsorption complexes were quantified and their dependence on the adsorption site was analysed. Some of the studied species have distinguishable vibrational parameters at different adsorption sites of the model nanoparticle, making spectroscopic characterization of respective adsorption complexes possible. *Finally*, the adsorption and the partial hydrogenation of 1,3-butadiene (BD) on two different configurations of the Pd<sub>n</sub>/Ni<sub>m</sub>(111) multilayers has been studied. The most stable adsorption sites are dependent on the substrate composition and on the inclusion or not of spin polarization. The magnetization of the Pd atoms strongly modifies the adsorption energy of BD and its most stable adsorption mode. On the other hand, as a consequence of BD adsorption, the Pd magnetization decreases. All calculations were performed using the VASP method in the framework of density functional theory (DFT).