Hazar GUESMI

CNRS I Researcher

Charles Gerhardt Montpellier Institute

https://www.icgm.fr/hazar-guesmi/

Biography

Hazar GUESMI earned her Ph.D. degree in Materials Science at the University of Aix-Marseille III, France (2005). She performed her doctoral work under the supervision of Prof. Müller and Dr. Tréglia at the "Centre de Recherche de la Matière Condensée et des Nanosciences" in Marseille, where she studied the adsorption mechanisms on Si surfaces. From 2005 to 2006 she worked as assistant professor at the university "Pierre et Marie Curie", Paris VI and she developed her research activity on gold nanodots in the Institut des NaonoSciences de Paris. In September 2006 she obtained a Post Doctoral grant via the European Network of Excellence and she worked for two years on the modeling of DeNox reaction in zeolites at the Institut Charles Gerhardt in Montpellier. In October 2008 she was appointed as a permanent CNRS researcher in the "Laboratoire Réactivité de Surface" in Paris (Sorbonne université) and after four years she moved to the ICGM. Currently, she is member of the Theoretical Physical Chemistry and Modeling department at the "Institut Charles Gerhardt" where she develop computational and theoretical studies on surface science and heterogeneous catalysis.

Predicting realistic shape and structure of nano-catalysts under working conditions: Are we there ?

Metallic and bimetallic nano-catalysts typically operate under high-pressure and high-temperature conditions, and this reactive environment may substantially influence the structure and the surface composition and therefore the reactivity of these nano-materials. Theoretical studies of catalytic properties are often investigated on model systems (extended surfaces and/or small nanoparticles) where no account is taken for the possibility that the catalyst surface composition can be modified after the gas exposure [1]. This is a serious drawback that may prevent reliable description of the catalyst reactivity that mainly depends on the configuration of the surface. Nowadays, modeling the equilibrium structure and the shape of nano-catalysts in a “realistic” reactive environment is still a barely studied subject and remains an extremely challenging task.

Recent works in the group were focusing on the prediction and the study of the structural changes of metallic and bimetallic systems under reactive gas and on their related catalytic properties [2-5]. Different theoretical approaches based on Density Functional Theory (DFT) calculations, Monte Carlo (MC) and ab-initio molecular dynamic (AIMD) simulations were developed to predict “realistic” catalytic surfaces under reaction conditions. In this talk, I will present an overview of our main recent results and I will focus on the advantages and limitations of the developped theoretical approaches.

Keywords:

Structural dynamics; heteregenous catalysis; DFT and molecular dynamics; Surfaces and nonparticles; Effect of reactive gas

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