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Multidisciplinary theoretical studies of small nanostructures of carbon compounds for multiplepurposes

FernandoRuette
Instituto Venezolano de Investigaciones Cientificas (IVIC), Venezuela

Carbonaceous materials, based on polyaromatic hydrocarbons (PAH), have multiple applications particularly on: atmospheric chemistry, heavy oil components, interstellar chemistry, liquid crystals, carbonization chemistry, catalysis, electronic components, etc. In this presentation, several interactions between radicals with a PAH (coronene molecule) have being studied: (a) model aging of black carbon (BC) produced in air pollution [1]; (b) formation of molecular species on carbonaceous material of the interstellar medium (ISM) [2]; (c) the metal and metal oxides species formed on pyrolytic graphite platform (PGP), used in electrothermal atomic absorption spectroscopy (ETAAS) [3]; (d) metal supported on graphene for the catalysis of olefin hydrogenation [4]. For modeling the above mentioned systems, quantum chemistry calculations at DFT level, parametric, tight binding, and Monte Carlo techniques were employed.

(a) Potential energy surfaces for •OH reaction with coronene as model of BC were evaluated to explain the aging of BC. It means, BC destruction in atmosphere is simulated by the breaking of C-H and C-C bonds after multiple interactions with •OH with the formation of CO_2 plus H_2O. This aging process goes through on the edge surface oxidation with the formation of OH, C=O, and COOH groups. The increase of the surface hydrophilicity was analyzed by using PM6 and DFT-D, explaining water condensation [1].

(b) Several studies of molecular formation in the ISM were carried out for the formation of H_2, H_2O, CH_4, NH_3 molecules after multiple hydrogenations by (Eley-Rideal (ER) mechanism). Events associated with these processes have been studied with the calculation of chemisorption, diffusion, desorption, and surface reaction barriers [2]. The temperature desorption spectrum (TDS) of H2 on graphite is simulated with a Monte Carlo approach using calculated barriers of each event with DFT. A very good theoretical and experimental matching is obtained. The effect of multiple layers of graphene and ionization (charge effects) were also analyzed.

(c) Comparison between X-ray photoelectron spectra (XPS) and theoretical stability of possible Mo species on a model of pyrolytic graphite at different stages of the ETAAS process was performed [3]. The interpretation of XPS in different regions of the PGP indicates the migration of MoxOy species far from the center region. It was found that very stable oxides on the edges of the graphite are formed, then reductions of these species are feasible because are thermodynamically favored. Carbide formation on the dehydrogenated sites is responsible for observed species at ETAAS.

(d) Highly dispersed nanocatalyst synthetized by metal deposition on small graphenes was theoretically modeled [4]. Metallic nickel chemisorptions on multiple sites yield a very active catalyst for hydrogen activation. The interaction with ethylene is analyzed on different sites. Results show that the activation barrier for ethylene hydrogenation is very low. A novel catalyst is proposed for hydrogenation of hydrocarbons.

One may conclude that carbonaceous surfaces have multivariate technological applications, particularly, for recombination of radical species on their surfaces.

fruette@ivic.gob.ve

SAR156497 an exquisitely selective inhibitor of aurora kinases

Jean-Christophe Carry
Sanofi, France

The Aurora family of serine/threonine kinases is essential for mitosis. Their crucial role in cell cycle regulation and aberrant expression in a broad range of malignancies have been demonstrated and have prompted intensive search for small molecule Aurora inhibitors. Indeed, over ten of them have reached the clinic as potential anticancer therapies. We will report the discovery and optimization of a novel series of tricyclic molecules that has led to SAR156497, an exquisitely selective Aurora A, -B and -C inhibitor with *in vitro* and *in vivo* efficacy. We will also provide insights into its mode of binding to its target proteins from X-Ray data, which could explain its selectivity.

jean-christophe.carry@sanofi.com