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Role of the catalyst in the synthesis of carbon nanotubes

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The formation of single-wall carbon nanotubes requires the presence of a metal catalyst whatever the technique used. To understand their growth mechanism, we have initiated a theoretical study in order to simulate the segregation and the self-organization of the carbon atoms at the surface of metallic nanoparticles. We have developed a semi-empirical model based on tight-binding method to describe binary systems. A minimal basis is used to obtain a transferable tight-binding parametrization of the C-C, Ni-Ni and Ni-C interactions applicable to binary systems. Using this model, we have investigated the first stages of the nucleation process with Monte Carlo simulations in the grand canonical ensemble and demonstrated the role played by the metal in the dissolution-segregation process of carbon atoms [1].

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Phosphonate-based hybrids: from structural aspects to biological applications

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X-ray diffraction has largely contributed to the development of metal phosphonate chemistry, as a direct or indirect method. We will show the significant structure directing role of the organic moiety in this class of organic-inorganic hybrid materials [1]. From our experience in the coordination chemistry of phosphonic acids, we were able to develop applications of metal phosphonates in the field of catalysis and biotechnologies as well. For this latter aspect, we will report the design of a novel drug delivery system, based on the surface modification of calcium phosphates, using gem-bisphosphonic acids [2]. The resulting biomaterials show promising in vivo results for local osteoporosis treatments.

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