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Modification of magnetic properties of iron clusters by doping and adsorption

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Electronic and geometrical structure of neutral and charged iron clusters Fe_n, Fe_n^-, and Fe_n^+ (n = 2-20) will be discussed. Computational results will be compared to experimental data, in particular, to the recent data obtained from the magnetic moment measurements of Fe_n^+. We consider iron cluster oxides, single Fe atom oxides FeO_n for n up to 18, and FeX_n superhalogens. We present the results of computational simulations of gas-phase interactions between small iron clusters and OH, N_2, CO, NO, O_2, and H_2O. Competition between surface chemisorption and cage formation in $Fe_{12}O_{12}$ clusters will be discussed. The magnetic quenching found for $Fe_{12}O_{12}$ will be qualitatively explained using the natural bond orbital analysis for Fe_2O_2. Special attention will be paid to the structural patterns of carbon chemisorbed on the surface of a ground-state Fe_{13} cluster.

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Biointerface dynamics - Multi scale modeling considerations

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Complex multi-scale interactions among immobilized cell aggregates and the surrounding matrix within the Ca-alginate microbeads at various space scales: (1) at the bio-interface, (2) within the perturbed boundary layers around the cell aggregates, (3) within the microbead parts (consists of a few cell aggregates with perturbed matrix boundary layers and un-perturbed matrix parts) and (4) within the microbead as a whole are considered theoretically based on thermodynamical and rheological approaches. The irreversible nature of the matrix structural changes considered at various space scales is modeled at two time scales i.e., a long time scale (cell growth time), and a short time scale (cell rearrangement time). A comparison of various modeling approaches shed light on the essential mechanism of the structural changes of the matrix sub-system caused by cell rearrangement and growth. The mechanism is connected with energetically perturbed cell states caused by the interactions with the polymer matrix at the bio-interface. These cell states and the rate of their changes induces perturbation of the matrix state at the interface and within the boundary layers around the immobilized cell aggregates. The mechanisms of structural ordering of both sub-systems induce time delaying effects which lead to the anomalous nature of energy transfer and dissipation through the microbeads. The phenomenon could be related to the micro-environmentally restricted cell growth which has a great practical importance in prediction and optimization of various bio-processes such as: (1) mechanically suppressed tumor growth, (2) cell growth and products secretion, (3) artificial organs formation.

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