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Monofluoride electronic structure material for laser cooling applications

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Monofluorides are presently advanced materials that are being considered as interesting candidates for laser cooling and ultracold trapping experiments. The later have different applications in the domains of precision spectroscopy, quantum computing, and nanolithography. We present in this work theoretical ab-initio calculation of the ground and excited electronic states of the mono fluoride compound material BeF. We use Complete Active Space Self Consistent Field (CASSCF) method with Multi Reference Configuration Interaction (MRCI), toinvestigate the corresponding molecular potential energy and electric dipole moment curves (variation as a function of internuclear distance). We deduce values of the corresponding spectroscopic constants: The internuclear distance Re, the harmonic frequency ωe, the rotational constants Be, the electronic transition energy with respect to the ground state Te, the Eign values Ev, the abscissas of the turning points Rmin and Rmax, the rotational constants Bv, and the centrifugal distortion constants Dv. Results agree well with experimental data.

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Biological effects and some aspects of practical applications of nanomaterials

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Nanosized materials have potential of practical application in number of research fields, in industrial production and in everyday life. However, at nanoscale level they acquire new properties and therefore may become biologically very active. The biological toxicity of novel nano-particles is a key issue which has to be clarified before their full integration in everyday life. In this report the existed approaches for the determination of the biological effects of these types of substances are presented. Moreover, the positive and negative effects of nano-materials are given. The main attention is given characteristics of the approaches used at the express estimation of the total toxicity with the application of bacteria, Daphnia and plants with the express control of the level of bio- and enhanced chemi-luminescence, the energy of seed germination and efficiency of the photosynthetic apparatus of plants with the application of the special "Floratest" biosensor. In additional to that it is analyzed in detail cytotoxicity and genotoxicity of number of nano-materials. Using of the mentioned above methodical approaches three aspects of biological effects of such nano-materials, as: a) nano-particles ZnO, AgO, FeO, TiO2 and others, b) their colloidal substances and c) number of nano-composites, are considered. Namely, there is analyzed: a) biocidal activity (nano-particles); b) improvement of the nutrition of plants at the special conditions and c) a class of heterogeneous catalysts (as novel Nb(V)-containing saponite clay) which are able to promote selective oxidation of toxins into non-toxic products that is very important in case of disposal of chemical weapons.

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