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Doubly-charged negative ion of C_{60}

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Synopsis An electronic structure of the negative ion C_{60}^{2-} has been studied. It is found that in the first approximation of the variational method (when a trial wave function of the extra electrons is a product of one-electron functions) the total energy of the system is negative and that the second electron affinity (EA) of the C_{60} molecule within the utilized model potentials is about 1 eV. The photodetachment cross sections of the C_{60}^{2-} ion have been calculated as well; they are found to exhibit two different threshold behaviors with their values being of the same order as the photodetachment cross sections of atomic negative ions with the same EA.

An electronic structure of the doubly-charged negative ion C_{60}^{2-} has been studied by a variational method. It was assumed that the closed-shell C_{60} molecule is spherically symmetric, and the interaction of the added electron with the molecule is described by a potential $U(r)$ having in the jellium model [1] the Lorentz-like profile

$$U(r) = -U_0 / [(r-R)^2 + d^2]$$

The parameters of $U(r)$ (the fullerene radius R, well depth U_0 and thickness d) are such that upon solving the wave equation with this potential for a single electron the first EA of the C_{60} molecule agrees with the measured value of ε_1=2.65 eV [2]. At the limit $d \to 0$ this potential is transformed into the Dirac-bubble potential [2]. It is assumed that in the $1s^2$ ground state of the system C_{60}^{2-} both electrons are in a state with zero orbital angular momentum and antiparallel spins. Firstly, the energy of the ground state of the system C_{60}^{2-} was estimated within the framework of perturbation theory, with the wave function of the electron pair represented as a product of one-electron functions. The obtained total energy of the electrons E, confined within the potential well $U(r)$ with thicknesses varying from d=0 to 1.5 atomic units (au), was found to be negative. Consequently, the existence of the doubly-charged negative ion of C_{60} within the Lorentz- and Dirac-bubble potential models is quite acceptable.

Secondly, the total energy E and the electronic wave function φ of the ground state of the doubly-charged negative C_{60}^{2-} ion were obtained by a direct variational method. A trial wave function of the extra electrons was written as a product of one-electron functions of the C_{60}^{-} negative ion having the asymptotically corrected behavior inside and beyond the fullerene bubble [2].

It has been shown that the total energy $E(\beta)$ as a function of the variational parameter β reaches its minimum at β_0=0.4269 au, which corresponds to the energy $E(\beta_0) \approx$ -1.59 eV. So, the second EA of the C_{60} molecule is equal to $\varepsilon_2 = \varepsilon_1 + E(\beta_0)$=1.06 eV, which is rather close to the results of other estimations [3].

Note that the long-lived doubly-charged carbon cluster anions C_{60}^{2-} in the gas phase have been reported from both sputtering of a graphite surface by Cs^+ ions [4] and the laser desorption from a surface covered with the neutral C_{60} molecules [3].

The photodetachment cross-sections $\sigma(\omega)$ of C_{60}^{2-} have also been calculated using the wave functions $\varphi(\beta_0)$. Near threshold $\sigma(\omega)$ is found to exhibit peculiar and interesting behavior. The first cross section accompanied by the transformation of the doubly-charged negative ion into a singly-charged one is exponentially small near the process threshold. The second cross section corresponds to the photodetachment of a singly-charged ion; it increases at the threshold as a power function of the kinetic energy of the photoelectron. These cross sections are of the same order as the photodetachment cross sections of atomic negative ions with the same EA.

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