# Correlation-bound states of C_{60}^- anion

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We report on large-scale *ab initio* electronic structure calculations for the *bound* electronic states of the C_{60}^- anion. C_{60} (buckminsterfullerene) is known to be a strong electron acceptor, able to capture one or several electrons [1]. Among the C_{60}^- species it is only the ground state $^2T_{1u}$ that has been thoroughly studied from both experimental and theoretical point of view [2]. It is however very little known to date about other, less bound (excited) states of C_{60}^-. Are there such states at all and how many are there? In fact, identifying such states in C_{60}^- represents a big challenge. The main obstacles here are the large number of electrons (241 valence electrons) and, what is more crucial, the necessity of a proper treatment of electron correlation effects. These effects turn out to be strong already in neutral C_{60} and "go off scale" in the C_{60}^- anion. It is in fact the electron correlation (disperse-type) effects that were found to bind the extra electron in the C_{60}^{-*} anion excited states. These states are therefore termed *correlation-bound* states.

Using the highly accurate coupled cluster (EOM-EA) method we demonstrate that C_{60}^- possesses at least three correlation-bound, excited electronic states. These are $^2T_{1g}$, $^2T_{2u}$ and ^2A_g in order of decreasing the electron binding energy (see the figure below). Here it is noteworthy that ^2A_g was only very recently predicted to exist (being bound) [3] whereas the $^2T_{2u}$ state has been unknown to date. In the present work we focus on characterization of the above states in terms of their binding energies as well as with regard to their electronic structure, in particular the spatial distribution of the extra electron. To this end we employ the natural bond occupation analysis based on the computed one-electron densities.
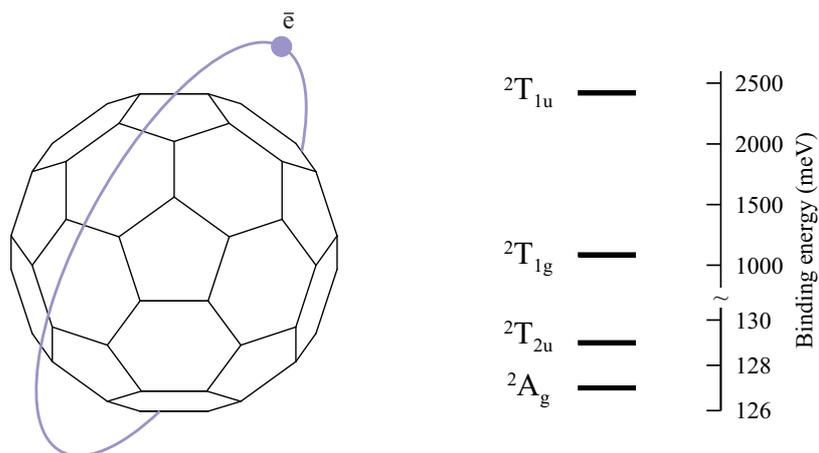
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