Modelling doubly charged fullerene clusters

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Calculations at the electronic structure level of systems involving several hundreds of electrons are quite demanding and become easily computationally inaccessible for post-Hartree Fock methods. Density functional theory (DFT) provides a possibility to calculate large systems without neglecting electrons.

Here we present a DFT study on doubly charged fullerene clusters to investigate their stabilities with respect to Coulomb explosion. In experiments involving charge transfer reactions from He^{*-} [3] as well as highly charged Xenon cations to neutral clusters of fullerenes, both dianions [2] and dications [3] have been observed, respectively. For both negatively and positively charged systems the pentamer is the smallest fullerene cluster which was detected in experiments. We explore the stability of small fullerene clusters and selected fragmentation pathways with DFT methods and compare these results to simple, heuristic models [4]. The results and conclusions of our study will be presented and an outlook on the stability of doubly charged adamantane clusters will be given.

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