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Title: Ab initio Investigation of Electronic Structure of Endohedral Fullerenes and Prismane Formation

Authors: Equbal, Asif (/jspui/browse?type=author&value=Equbal%2C+Asif)

Keywords: Ab initio
Chemistry

Issue Date: 5-Jun-2013

Publisher: IISER M

Abstract: Ab initio and DFT calculations have been carried out for B2@C60, O2@C60 and Ge2@C60 to study the influence of the fullerene cage on the relative stability of the triplet and singlet states of the diatomic molecules. For O2@C60, the relative energy of the encapsulated singlet and triplet states is similar to that of the relative energy of the singlet and triplet states of O2 when it is free. In the case of B2@C60, it was found that the energy difference between B2@C60 (triplet) and B2@C60 (singlet) is slightly larger in magnitude, suggesting that the triplet state is slightly more stabilized inside the cage than in free B2. However, the energy gap between the triplet and the singlet state of Ge2@C60 is significantly different from that of free Ge2 and it shows a dependence on the orientation of Ge2 in C60. All DFT calculations except the one using M06-2X suggest that Ge2@C60 is more stable in the singlet state in the D5d orientation and the triplet state is more stable in the D3d orientation. The electron density is different around a hexagonal ring when compared to a pentagonal ring in C60, giving rise to different interactions for these two orientations. There is a spin cross over as Ge2 rotates from D5d to D3d orientation. No such spin cross over is observed in B2 and O2 presumably because they have shorter bond lengths and there is very little interaction between them and the inner wall of the cage. In the case of silicon substituted benzene dimers, it is shown that the stability of the dimer increases with an increase in the number of Si atoms. This is presumably because with an increase in the number of Si atoms, the number of cyclobutane rings in the prismane decreases and there is an increase in the number of silicon atoms getting energetically favourable sp³ hybridization. The trends observed for Ge-substituted benzene are similar to those observed for Si-substituted benzene. Capped fullerenes are unstable when compared to isolated benzene and C60 fullerene. But the instability is less when compared to the instability in the case of [6]-prismane formation. An increased stability of the capped fullerene is noticed, when the hydrogen atoms in the benzene ring are replaced by the more electronegative fluorine atoms.

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