

Structural and electronic properties of the fullerene isomers of Si_{38} : A systematic theoretical study.

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(Dated: February 21, 2007)

I. SUPPORTING INFORMATION

A. Distributions for the 38:9 isomer (optimum)

For completeness we present here the corresponding figures of the distributions shown in the paper, for the optimum energetically isomer (i.e. isomer 38:9). As one can see, there is nothing particular in local planarity, pentagon and hexagon angle distributions or hybridization which would pick out isomer 38:9 uniquely from the others.

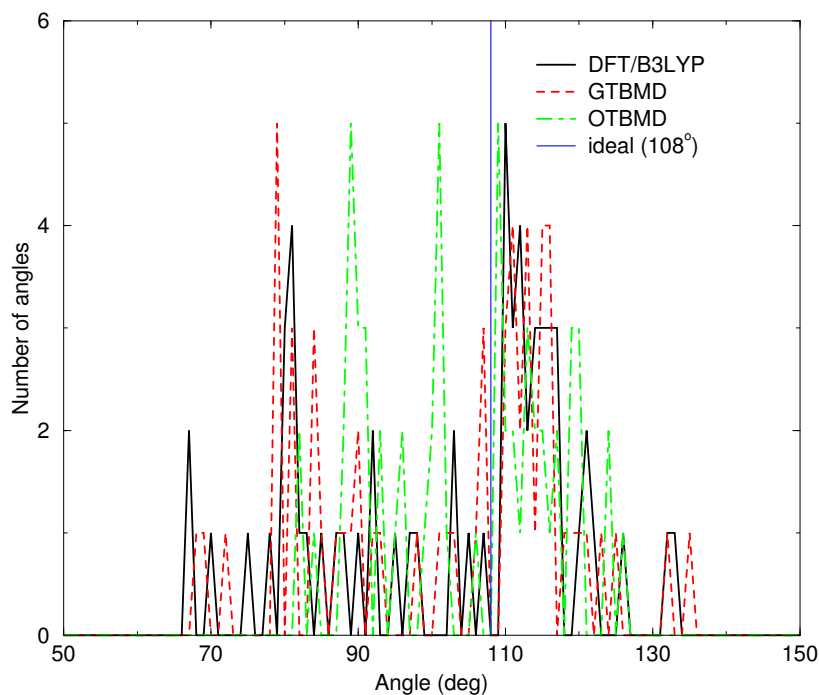


FIG. 1: Distribution of the pentagon angles for the 38:9 isomer for the : (I) DFT/B3LYP (solid line), (II) GTBMD (dashed line) and (III) OTBMD (dot-dashed line) calculation.

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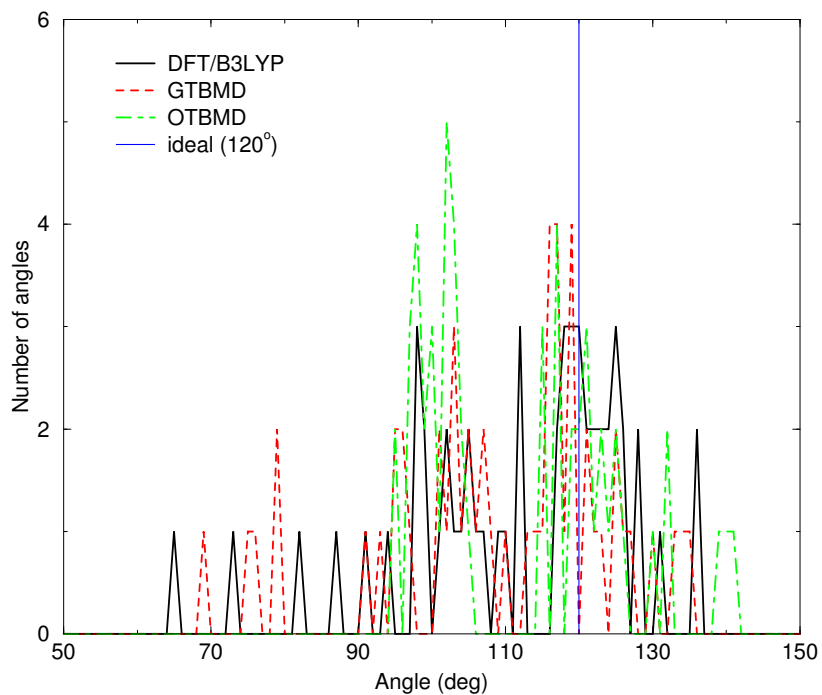


FIG. 2: Distribution of the hexagon angles for the 38:9 isomer for the : (I) DFT/B3LYP (solid line), (II) GTBMD (dashed line) and (III) OTBMD (dot-dashed line) calculation.

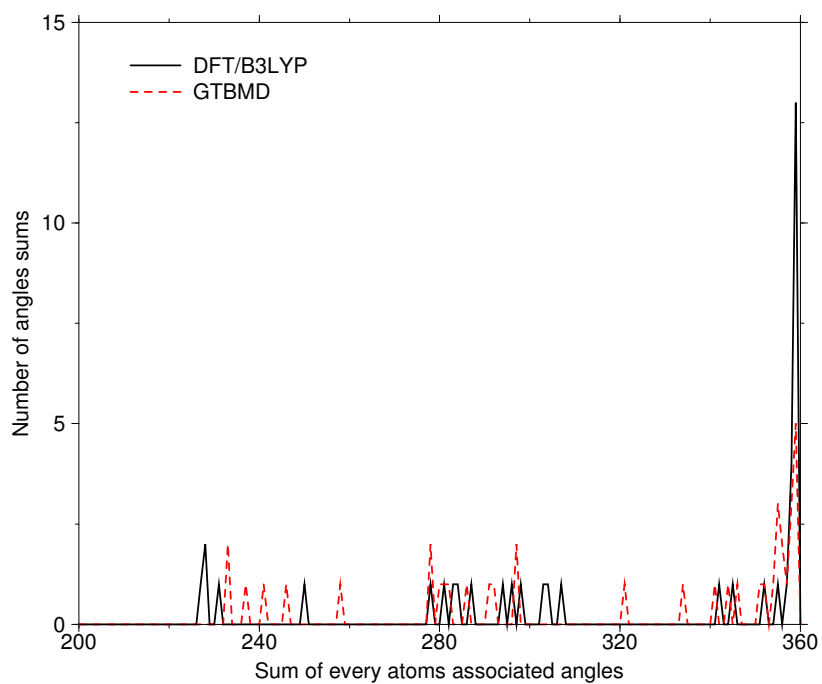


FIG. 3: Distribution of the angle sums associated with every atom, for the 38:9 isomer, obtained with (a) DFT/B3LYP (solid line), and (b) GTBMD (dashed line).

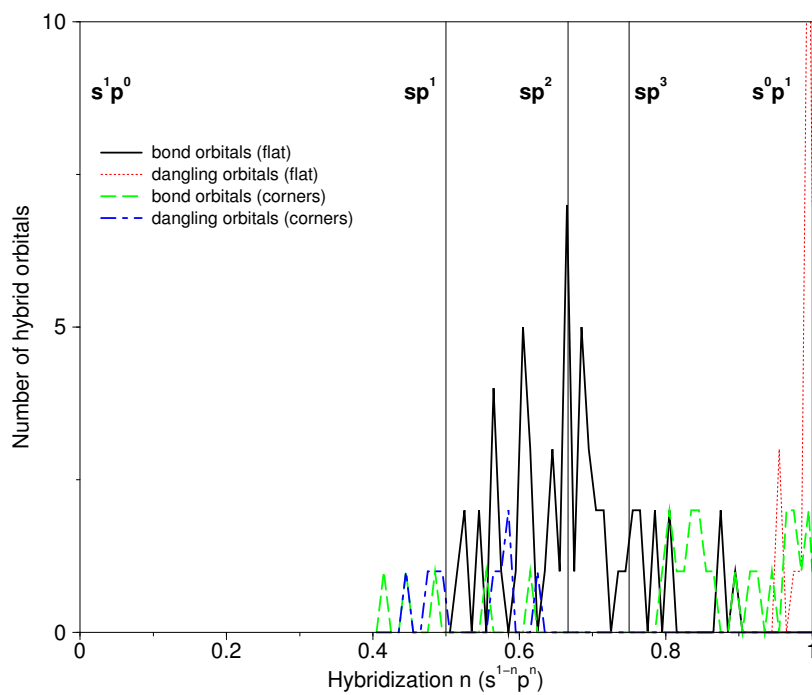


FIG. 4: Distribution versus n of (a) the three hybridized bond orbitals for near-planar the atoms (solid line), (b) the dangling orbital for the same atoms (dotted line), (c) the bond orbitals for the atoms at sharp corners (dashed line), (d) the dangling orbitals for the same atoms (dot-dashed line), for the 38:9 isomer (OTBMD method).