Center for Computational Sciences, University of Tsukuba
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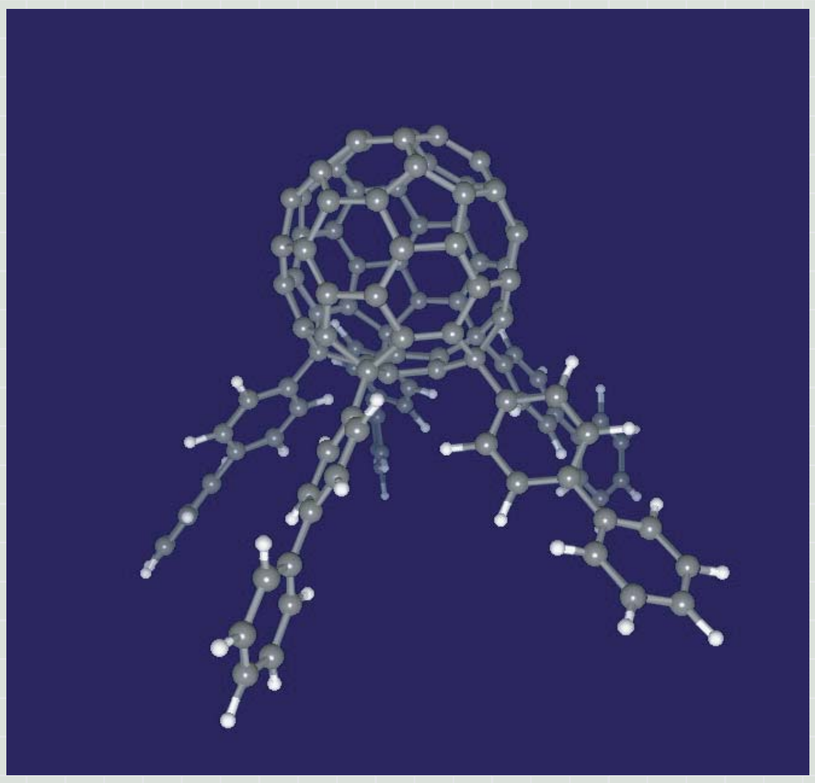
Computational Material and Life Sciences (1)

Nanocarbon shuttlecock



Recently, a new form of C_{60} derivatives with conical shapes has been synthesized under controlled modifications of C_{60} by attaching aromatic molecules. The derivatives consist of C_{60} at the apex and five phenol groups which are attached to five carbon atoms surrounding the one of the twelve pentagons in C_{60} so that its shape is a nanometer-scale badminton "shuttlecock". It has been also found that the shuttlecock molecules are self-assembled into solid or liquid-crystal phases, where the shuttlecocks are stacked in a head-to-tail way forming one-dimensional columns which are in turn arrayed in a pseudo-hexagonal packing.

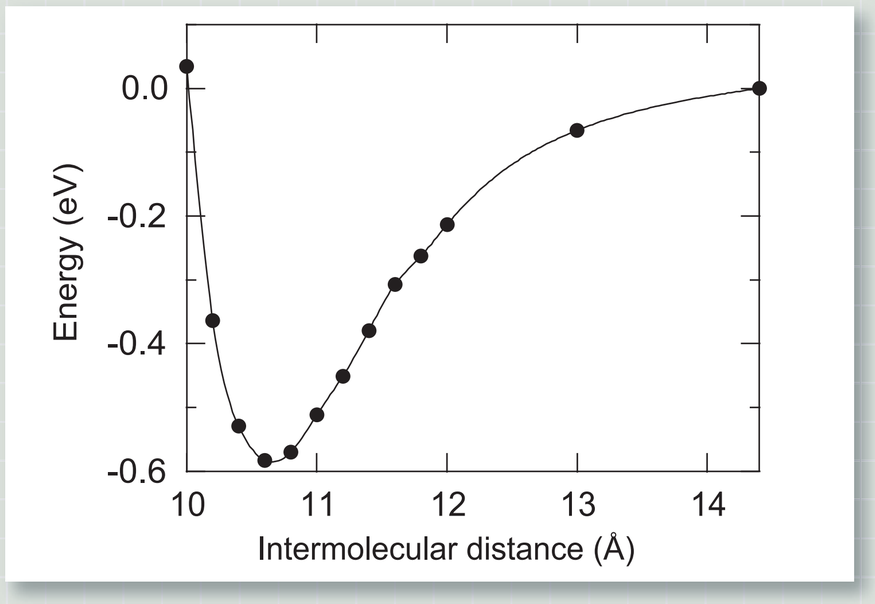
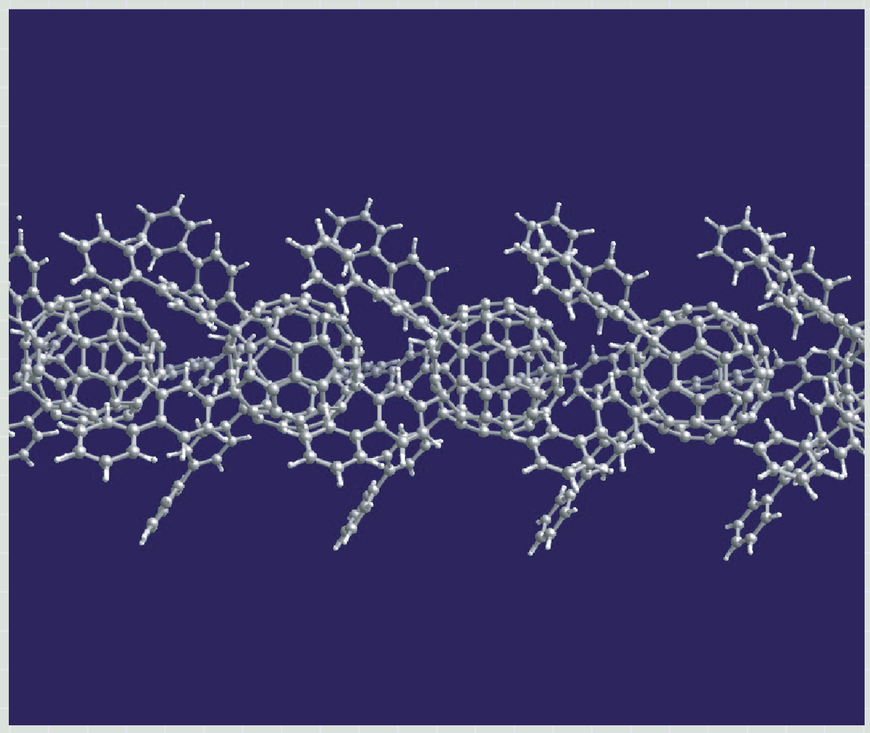
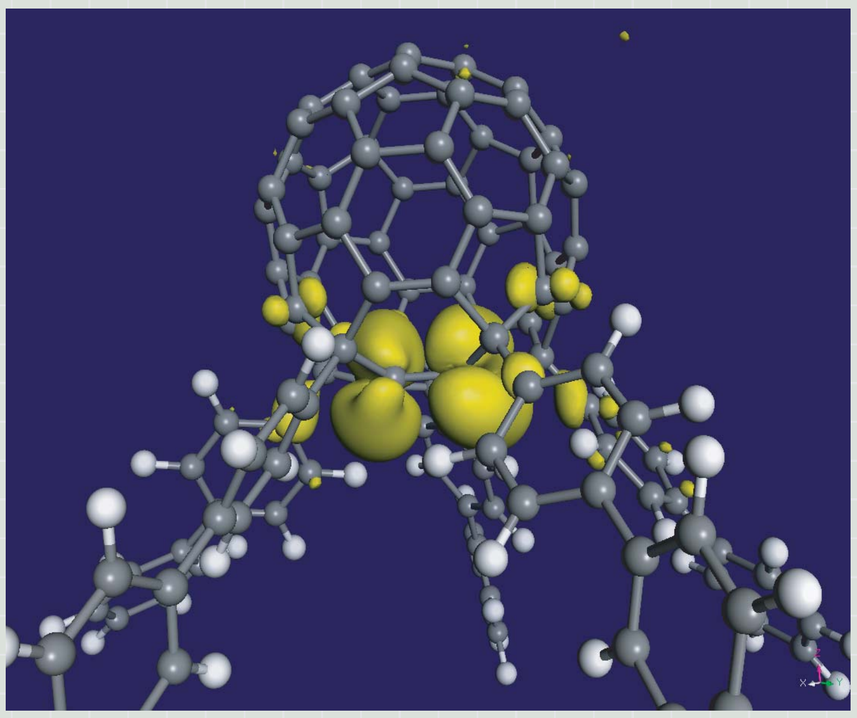


Figure shows the total energy of the C_{60}-(biphenyl)$_5$ chain versus intermolecular distance along with the optimized structure. The optimum intermolecular distance is 10.6 Å, which is greater than that (10 Å) in the solid C_{60}. The large distance between C_{60}s is due to the steric hindrance between the C_{60} apex of the shuttlecock and the H atom attached to a pentagon surrounded by the five biphenyls in the adjacent shuttlecock. In addition to this effect, van der Waals interaction between the biphenyls and the C_{60} also results in the large intermolecular distance.





The attachment of the molecules to C_{60} effectively divides the spherical **π** electron network into two segments; C_5 ring (cyclopentadieny) and C_{50} cage. The dissection results in narrow bands (with width ~ 50 meV) around the Fermi energy for the C_{60}-(biphenyl)$_5$. The narrow band results in the localized spin on each C_5 surrounding by the "feathers" in the shuttlecock.