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Computational Search for Novel Endohedral Fullerenes[1] LUIS BASURTO, TUNNA BARUAH, RAJENDRA ZOPE, University of Texas at El Paso
— Carbon fullerenes are often used as electron acceptors due to their large electron affinity, low reorganization energy and three dimensional charge transport property. The open circuit voltage in organic photovoltaics is known to be related to the energy difference of the highest occupied molecular orbital (HOMO) energy of the donor and the lowest unoccupied molecular orbital (LUMO) of the electron acceptor. The use of endohedral fullerenes as electron acceptors offers an alternative way to manipulate its LUMO levels by varying the encapsulating unit. In recent years a few donor-acceptor complexes with endohedral units have been reported. We have recently designed a set of computational tools to search for stable endohedral fullerenes. Using this toolkit, we have optimized all 31924 isomers of C80fullerenes. Using the lowest 3000 and a few other promising candidate structures a set of 22000 endohedral complexes of Sc3N@C80 and 10000 complexes of Sc4O2@C80 was constructed. This set was subsequently optimized at PM6 level and the lowest few geometries were relaxed at the PBE-GGA level within DFT. These calculations confirm previously assigned fullerenes geometries and report a few new low energy isomers. This procedure is extended to search for novel endohedral fullerenes.

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