

## Endohedral fullerenes for organic photovoltaic devices

Organic solar cells draw a lot of attention of many research groups located around the world. The reasons include significant progress in the design of p-type semiconductor materials (e.g., conjugated polymers) for organic solar cells particular, photovoltaic devices based on conjugated polymers exhibit high certified power conversion efficiencies of up to >17 ...

Here, we present a means of addressing the low voltage output by introducing novel trimetallic nitride endohedral fullerenes (TNEFs) as acceptor materials for use in photovoltaic devices. TNEFs were discovered in 1999 by Stevenson et al.; for the first time derivatives of the TNEF acceptor, Lu(3)N@C(80), are synthesized and integrated into OPV ...

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Endohedral fullerenes were reported soon after the discovery of C 60 [22], [23], but their low synthetic yields and inefficient separation methods limited the ability to fully investigate their properties 1999, Dorn et al. serendipitously revolutionized the endohedral fullerene field, with the discovery of the first cluster endohedral fullerene, Sc 3 N@I h-C 80 [24].

6.1 Functionalized Fullerenes for Photovoltaics/Solar Cells. The C 60 fullerene is a unique structure that is electron-deficient and can act as an electrophile in various organic syntheses. One of the most exciting applications of functionalized fullerenes is in the field of photovoltaics or solar cells.

One of the most attractive properties of fullerenes is their cage-like structures, capable of acting as robust nanocontainers for other species such as metal ions or metallic clusters. Fullerenes with such host-guest structures are named as ...

Organic photovoltaic (OPV) devices have incorporated fullerenes as efficient electron acceptors and conductors for many years with promising results. 25 Although many OPV devices with fullerenes as electron acceptors have been reported, only one example using a cluster containing endohedral has appeared. 26 Bis-functionalized fullerenes have ...

The performance of organic photovoltaic (OPV) material systems are hypothesized to depend strongly on the intermolecular arrangements at the donor:fullerene interfaces. A ...



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Condensed Fullerene. Fullerenes in Photovoltaics Fullerenes in Biosciences Small-Cap Fullerenes. Introduction. Twenty-five years ago, it was discovered that carbon vapor preferentially condenses into an exceedingly stable cluster with 60 carbon atoms (C 60), and it was hypothesized that the 60 atoms were arranged as the vertices of a truncated icosahedron, aka ...

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Compared with the empty fullerenes, EMFs can act as promising materials for organic photovoltaic devices because of the doping of metallic species, which normally results in high lowest unoccupied molecular orbital energies. Likewise, our group ... Endohedral fullerenes. Chem. Rev., 113 (2013), pp. 5989-6113. Crossref View in Scopus Google ...

Fullerenes are spherical carbon molecules consisted of only pentagonal and hexagonal carbon rings, with I h-C 60 and D 5h-C 70 (nomination following the spiro algorithm proposed by Fowler and Manolopoulos []) as the most abundant compounds [].Endohedral metallofullerenes (abbreviated as EMFs) are generated by encapsulation of metallic clusters ...

Fullerenes for organic photovoltaics OPVs: an introduction ... the weaker photoluminescence quenching which was registered for the endohedral containing devices results in less efficient charge carrier generation, and hence lower J SC. This might also be linked to an intramolecular electron exchange that competes with the donor-to-acceptor ...

So far, one of the fundamental limitations of organic photovoltaic (OPV) device power conversion efficiencies (PCEs) has been the low voltage output caused by a molecular orbital mismatch between the donor polymer and acceptor molecules. Here, we

The resulting compounds, known as endohedral fullerenes, have been proposed for various applications such as organic photovoltaic (OPVs) devices 1,2,3, antimicrobial activity 4, ... etc. Among the ...

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Here the influence that 1-(3-hexoxycarbonyl)propyl-1-phenyl-[6,6]-Lu3N@C81, Lu3N@C80-PCBH, a novel acceptor material, has on active layer morphology and the performance of organic photovoltaic (OPV) devices using this material is reported. Polymer/fullerene blend films with poly(3-hexylthiophene), P3HT, donor



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Tuning Conversion Efficiency in Metallo Endohedral Fullerene-Based Organic Photovoltaic Devices By Russel B. Ross, Claudia M. Cardona, Francis B. Swain, Dirk M. Guldi, Shankara G. Sankaranarayanan, Edward Van Keuren, Brian C. Holloway, and Martin Drees\* 1. Introduction In recent years organic photovoltaics, OPVs, have gained an

The endohedral metallofullerenes (EMFs) consist of fullerene trapping inside the cage 1, 2, 3 metal atoms or clusters of up to 4 metal atoms including also nonmetals such as C,N,O,S. [6][7] [8] [9 ...

During the past 2 decades, photoactive electron donor-acceptor dyads have drawn great attention of researchers, especially in the field of organic photovoltaics (OPVs) [] particular, fullerenes like C 60 and C 70 and their derivatives have been widely used as electron acceptors in OPVs, due to their low reorganization energies and high electron affinity [].

Endohedral fullerenes for organic photovoltaic devices. Russel B. Ross1, Claudia M. Cardona2, Dirk M. Guldi3, Shankara Gayathri Sankaranarayanan3, Matthew O. Reese4, Nikos Kopidakis4, Jeff Peet5, Bright Walker6, Guillermo C. Bazan5, Edward Van Keuren1, Brian C. Holloway2 and Martin Drees2\* ... The trimetallic nitride endohedral fullerenes ...

The Journal of Organic Chemistry 2023, 88 (7), ... Nonionic Sc3N@C80 Dopant for Efficient and Stable Halide Perovskite Photovoltaics. ACS Energy Letters 2019, 4 (8), ... A Theoretical Study on the Stability of PtL2 Complexes of Endohedral Fullerenes: The Influence of Encapsulated Ions, Cage Sizes, and Ligands.

Fullerenes are known to have different isomers, with C 60 having 1812 theoretically different isomers []. These isomers can have different symmetry, form, and energetic stability. An example of the different structures of the six most stable isomers of C 80 is shown in Figure 1, with D 5d and D 2 being the most stable and abundantly found isomers []. ...

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