On the formation of smaller p-block endohedral fullerenes: Bonding analysis in the E@C20 (E = Si, Ge, Sn, Pb) series from relativistic DFT calculations

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Experimentally characterized endohedral metallofullerenes are of current interest in expanding the range of viable fullerenic structures and their applications. Smaller metallofullerenes, such as M@C28, show that several d- and f-block elements can be efficiently confined in relatively small carbon cages. This article explores the potential capabilities of the smallest fullerene cage, that is, C20, to encapsulate p-block elements from group 14, that is, E = Si, Ge, Sn, and Pb. Our interest relates to the bonding features and optical properties related to E@C20. The results indicate both s- and p-type concentric bonds, in contrast to the well explored endohedral structures encapsulating f-block elements. Our results suggest the E@C20 series to be a new family of viable endohedral fullerenes. In addition spectroscopic properties related to electron affinity, optical, and vibrational were modeled to gain further information useful for characterization. Characteristic optical patterns were studied predicting a distinctive first peak located between 400 and 250 nm, which is red-shifted going to the heavier encapsulated Group 14 atoms. Electron affinity properties expose different patterns useful to differentiate the hollow C20 fullerene to the proposed p-block endohedral counterparts. © 2017 Wiley Periodicals, Inc.

carbon

DFT

endohedral

fullerene

main group

Carbon

Electron affinity

Optical properties

Affinity properties

Endohedral fullerene

Endohedral metallofullerenes

Endohedral structure

Endohedrals

Main group

Potential capability

Spectroscopic property

Fullerenes