Non-charge-separated states of endohedral/endocircular alkali carbon allotropes

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Carbon allotropes have complex electronic properties. By inserting a guest atom, such as an alkali metal, carbon allotropes can form donor-acceptor charge-separated states,[1,2] in which the alkali atoms are the donors and the carbon allotropes are the acceptors. Until very recently, the theoretical chemistry group at Heidelberg -- based on the state-of-the-art equation-of-motion coupled cluster method calculations -- found that these endohedral/endocircular systems can also form non-charge-separated states, such as those termed the caged-electron state,[3] split-electron state[4], and the encircled-electron state. [5] In some cases, these non-charge-separated states can actually be the ground state of the system. Due to their interesting electronic properties, these states may have application potentials.

Reference:

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[3] Y.-F. Yang, E. V. Gromov, and L. S. Cederbaum. Caged-electron states in endohedral li fullerenes. *J. Phys. Chem. Lett.*, 2019, 10, 7617.

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