عنوان مقاله:

DFT Investigation of structure, stability, NBO charge on Titanium—Nitrogen nanoheterofullerenes evolved from a small nanocage

محل انتشار:

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خلاصه مقاله:

In this DFT approach, we are performed geometrically and electronically properties of Ti—N nanoheterocages developed from C۲۰ fullerene with the molecular formula of C۲۰-۲nTinNn (n = ۱-۸), at B۳LYP/۶-۳۱۱++G**, M۰۶۲X/۶-۳۱۱++G**, B۳PW۹۱/۶-۳۱۱++G**, and B۳LYP/AUG-cc-pVTZ levels of theory. Based on the vibrational frequency analysis, except for C۴Ti۸N۸ structure, others are real minima and none deform as segregated open cage. Substituted doping C۲۰ to its C۲۰-۲nTinNn derivatives are caused different ΔEHOMO-LUMO values and conductivity, so that there is no uniformity between the ΔEHOMO-LUMO and n (number of substituting Ti—N units) and C۱۸Ti۱N۱ is found as the best insulated nanoheterofullerene, while C۱۲Ti۴N۴ is considered as the strongest conductive nanocage. The results show good reliability among polarizability, and ionization potential with n. Thermodynamic stability and aromaticity (NICS values at cages centers) decreases as n increases. As such, the strong ring current in C۱۸Ti۱N۱ becomes weak in other nanostructures studied under work because the pπ electrons are slightly shifted from Ti to N (and C) atoms also portions of valence electrons keep on localized over the N (and C) nuclei. Accordingly, on account of lack of N—N bonds and dispersion of eight Ti—N bonds in the symmetrical positions of cage, the C۴Ti۸N۸ species conserves the cage structure, showing the lowest dipole moment of ۰.۰۰ Debye and the lowest positive charge on Ti atoms (+۰.۵۲۶). Considering the least absolute value of hydrogen adsorption energy | −۱۸.۹ kcal/mol | and the highest positive charge on titanium heteroatom of C۱۸Ti۱N۱ (+۱.۲۶۹), it seems that C۱۸Ti۱N۱ is the best candidate for hydrogen storage.

کلمات کلیدی:

Heterofullerene, Stability, DFT, NBO, NICS