عنوان مقاله:

Electronic structures and stabilities of endohedral metallofullerenes TM@C۳۴ using DFT approach

محل انتشار:

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خلاصه مقاله:

Theoretical study of the electronic structure using, Density Functional Theory (DFT) calculations at the B۳PW۹۱/۶-۳۱G (d) level of theory have been employed to the TM@C۳۴ (TM =Ti, V, Cr, Mn, Fe, Co, Ni, and Cu) in order to investigate the geometries, electronic structures, binding energies, linear polarizability ⟨Δ ⟩, first order hyperpolarizability ⟨ ⟩, natural bonding orbital (NBO), was studied based on the "C۳۴" fullerene. The results found that the most stable structure is e(C۲). Minimal energy structures of each endohedral metallofullerene were obtained. Hybridizations were found between the Ti, V, Cr, Fe, Co, and Ni, ۳d valence orbitals and the "C۳۴" cage orbitals, while none was found between the Mn and Cu orbitals and the "C۳۴" cage orbitals. These findings were obtained with the preferential position of the metal atom inside the fullerene cage, i.e. these results are found suitable for the metal Mn and Cu orbitals present inside the fullerene cage. Natural bonding orbital (NBO) shows that the charges always transfer from the TM atoms to the "C۳۴" cage. In going from isolated TM atom to TM@C۳۴, the occupation of the ۴s orbital is strongly reduced. The introduction to TM to the empty "C۳۴"leads to more active NLO performance. The TM@C۳۴ (TM =Ti, V, Cr, Mn, Fe, Co, Ni, and Cu) interactions are characterized in terms of several theoretical parameters such as density of states (DOS), molecular electrostatic potentials (MEPs), non-linear optical (NLO) properties and . electrophilicity and thermodynamic properties were also performed at B۳PW۹۱/۶-۳۱G (d) level of theory

کلمات کلیدی:

C۳۴", DFT theoretical investigation, Endohedral metallofullerene, NLO and NBO analysis, structure, stability," thermodynamic properties