By using the hybrid density-functional (B3LYP/6-31G (d, p)) method, we study the atomic structures and electronic properties of endohedral C20 and C20 H20 cages and its ions with H2 and H3.

The energetics and geometrical consequences of encapsulating the hydrogen species inside the C20 and C20H20 cages, which were geometrically optimized without constraints, are analyzed. The change of cage volume of linear and triangular H3@C20 cage is increasing from the cation through the neutral till the anion, but the change of the volume of linear and triangular H3@C20H20 cage is reversed. The correction of BSSE calculations suggest that the sum of atomic charges of encapsulated hydrogen species of 3H and 2H in linear and triangular H3@C20 and H3@C20H20 and H2@C20 and H2@C20H20 cations is negative, implying that some electrons of cage flow to the encapsulated hydrogen species in their cations, but the encapsulated species in the cases of neutral and anion in linear and triangular H3@C20 and H3@C20H20 cages, are positive. In the case of anions, the electron flow of H3@C20 is 5 times larger than that of H3@C20H20 anions. The characters of sp2 and sp3 of C are the similar in the electron deficient case, but they are different in anions.