Abstract Submitted
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Study of the Ce@C_{82}endohedral fullerene[1] ZHIFAN CHEN, ALFRED Z. MSEZANE, Clark Atlanta University — Ce@C_{82} endohedral fullerene has been studied using the DFT, GW approximation and TDDFT. In the simulation of Ce@C_{82}, a Ce atom was added inside the C_{82}-C_{2v} isomer along the C_2 axis. The Ce atom can be moved along that axis to find the minimum energy of the system. Three electrons have been removed from the Ce atom and a -0.5 electron has been added to each C atom of the six-membered ring of the C_2 axis to make the system neutral. A geometry optimization for a total of 550 electrons has been performed under the generalized gradients approximation (GGA) with the PW91 exchange-correlation functional. All electrons in the core were explicitly included in the calculation. Valence electrons were described by a double numerical basis set. The results of geometry optimization suggest that the Ce atom is situated off center by about 1.79Å which is compatible with the X-ray diffraction pattern data of 2Å. The density of the states, and density of the electrons for the Ce@C_{82}fullerene have also been calculated in the DFT. The band gap of 0.06 eV was obtained by the GW approximation. The optical absorption spectra are evaluated using TDDFT, RPA, and BSE.

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