Density functional study of spin polarization on a carbon material with a hexagonal structure induced by iron atoms

ABSTRACT

We investigate the spin polarization of a non magnetic material, e.g., a carbon material made from ten C atoms forming a hexagonal structure with total spin S = 0, induced by a ferromagnetic material, e.g., two Fe atoms with a total spin S = 4. Based on the density functional theory, we calculate the total spin density of the system. Our preliminary results show that the total spin for the ten C atoms changes from S = 0 to S = 4, while the total spin of the two Fe atoms changes from S = 4 to S =0. These results seem to indicate that there is a promising possibility to induce spin polarization on a carbon material by Fe atoms.

Keyword: Carbon material; Density functional theory; Ferromagnetic material; Scanning tunneling microscopy; Spin polarization