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Electronic and Magnetic Properties of Silicon-Carbide Fullerenes-like Nanostructures. HUSSAIN ALATHLAWI, MUHAMMAD HUDA, University of Texas at Arlington — Silicon carbide (SiC) is an important material for extreme environment applications, such as high temperature, high pressure, high power, etc. In its bulk phase, it has more than 200 polymorphs. At the nanoscale, stabilized functional clusters are of particular interest. Experimentally, the C_{60} fullerene was found to be the most stable form of carbon. On the other hand, Si and C have similar valence electrons configurations, implying that Si and SiC could form similar fullerene structures. We will present our first-principles investigations of the $Si_{30}C_{30}$ fullerene-derived clusters. The calculation started from the Si_{60} fullerene; we studied different configurations of $Si_{30}C_{30}$ fullerene-like structures and relaxed them without any symmetry. The result has shown some Si-C and Si-Si double bonds in unpassivated structures. Also, the endohedral doping of fullerene with W atom and the clusters' magnetic properties will be presented. In addition, we choose the most spherical structure, with a high number of Si-C bonds, to show the magnetic properties for the endohedral doping of transition metal atoms (W, Ta, Fe, Nb, Hf). Finally, stabilities of these clusters' will be discussed.

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