Said Al Azar, J Nanomater Mol Nanotechnol 2018, Volume 9
DOI: 10.4172/2157-7439-C8-088

Electronic structure and formation energy of $TiCxH_2$-x alloys: DFT study

Said Al Azar
Middle East Technical University in Amman, Jordan

In this work, the electronic structure and formation energy of $TiCxH_{2-x}$ alloys (x=0, 0.25, 0.5, 0.75, 1) are investigated by performing density functional theory calculations. The total energy calculations showed that hexagonal close-packed (h.c.p) structure is more preferable and stable than cubic (f.c.c) one for $x \geq 1/2$. The results showed that for the cubic (f.c.c) structure, hydrogen atoms are occupied partially both octahedral and tetrahedral interstices while carbon atoms occupied only the octahedral interstices. On the other hand, the hexagonal close-packed (h.c.p) structure showed that the octahedral interstices are fully occupied by carbon and the tetrahedral interstices are partially occupied by hydrogen.

Biography

My research focuses on subjects central to study and investigate computationally, from an ab initio standpoint, the electronic and magnetic properties of new functional nanomaterials such as catalyst, topological insulators, Half-metallic etc. One of the most important interests for me is to construct and modeling calculations by the clustering solution. If there are a clustering solution and HPC technology in your department, I can use these facilities and pursue my research projects. Furthermore, I was attended many workshops and tutorials in High-Performance Computing (HPC)and computational physics, which was very interesting and useful for me. My experience and knowledge in ab initio packages such as Wien2k and abinit, OS operating systems and C/C++ and FORTRAN programming qualified me to be a computational physics researcher.

q_saed74@yahoo.com

Notes: