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Prediction of acenes electron affinity energy using TIM

Ali Asghar Khakpoor and **Bahare Agahi Keshe**
Islamic Azad University, Iran

Manufacturing the nanoscale components has faced some limitations, which is virtually impossible in many cases. Acenes are organic molecules that have received considerable attention in molecular electronics and nanoscale. Due to the important electronic properties of the family, many studies have been conducted on them. A molecular graph is a simple graph whose vertex is mainly made up of atoms in a molecule and the bonds between atoms are the graph edges. In chemical graphs, hydrogen atoms were removed and excluded. Moreover, the degree of each vertex is a maximum of 4 and all bonds between atoms are considered as single. Topological indices are defined based on graph theory. The first Zagreb index is one of the topological indices, which is defined as follows $M_1(G) = \sum_{u \in V(G)} d^2(u)$

Where u is a member of the graph vertices and d is its degree. The Electron Affinity Energy was calculated using Gaussian 09 software and the experimental data of references were compared with those mentioned in valid papers. Prediction of electron affinity energy has a very high accuracy through the first Zagreb index with $R^2 = 0.9988$.

Biography

Ali Asghar Khakpour received his B. Sc. in Applied Physics from Esfahan University, Iran, M. Sc. degree in Solid state Physics from the Esfahan University in Iran and ph.d in Nano Physics at Material and Energy Research Center (MERC) in Iran. He is currently a assistant professor in Islamic Azad University- Central Tehran Branch (IAUCTB). He is a member of the Iranian Crystallography Association (ICA) and Iranian Physics Society (IPS). He has a project in TiO2 thin film as a self cleaning material and have several project in nano structures. He is interested to nano physics, thin films, quantom mechanic and mathematical physic . He has co-authored 2 books and approximately and has published over 36 publications on various aspects of atomic physics, TiO2 thin film and nano-science.He is also a lecturer at since 1993 in Iran, teaching different subject in Physics.

Ali.khakpoor@iauctb.ac.ir

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