Electronic Letters on Science & Engineering 12 (2) (2016)
Available online at www.e-lse.org

Special Issue
BSW2016
Fifth Bozok Science Workshop: Nano Carbon Materials and Their Applications

Bozok Science Workshop 2016, Yozgat, April 28-29, 2016.

HF AND DFT ANALYSIS OF STRUCTURE AND ENERGETICS OF $Zn(H_2O)_n$ FOR n=1-10

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Abstract: Structural and energetic properties of water and metal doped water clusters have been interesting subjects [1,2]. In this study, size dependent changes of structural and energetic quantities of zinc-doped water clusters, $Zn(H_2O)_n$ n=1-10, have been investigated by using Hartree-Fock (HF) and Density Functional Theory (DFT/B3LYP and DFT/PBE) at 6-311++G(d,p) basis set [3]. The total and binding energies of the considered clusters have been calculated. Energies for the highest occupied molecular orbitals (HOMO) and the lowest unoccupied molecular orbitals (LUMO) have been computed and their energy gaps have been determined. Zn-doping affects the structural stability of the water clusters. Energetic and structural parameters have been analyzed as a function the number of the water molecules in the clusters and findings have been compared with each other for the selected theories.

Keywords: *Water Clusters, Zinc, HF, DFT.*

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ISSN 1305-8614