Proceedings
International Journal of Nanomaterials, Nanotechnology and Nanomedicine

Special Issue: NCNN-2014
(National Conference on Nanoscience and Nanotechnology - 2014)

A Density Functional Approach: Cationic Interaction in Polymer Systems

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First principle calculations based on density functional theory is performed to analyze the cationic interaction with the polyethylene oxide (PEO) based systems. The relaxed polymer structures are simulated, the analysis of partial density of states; density of states; bond lengths and the charge density distribution around interacting atoms is made. The structural and electronic properties of polymer systems are discussed; it takes into account of the cationic and anionic nature of the atoms of dispersed molecules.

Citation: *Rao BK, Verma ML (2015) A Density Functional Approach: Cationic Interaction in Polymer Systems. Int J Nanomater Nanotechnol Nanomed S: 105.*