BEST: International Journal of Humanities, Arts, Medicine and Sciences (BEST: IJHAMS)
ISSN (P): 2348-0521, ISSN (E): 2454-4728
Vol. 5, Issue 05, May 2017, 25-34

THEORETICAL STUDIES OF NANOSILVER AND PMMA-AGNANOCOMPOSITES BY GAUSSIAN 09 PROGRAM

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ABSTRACT

The theoretical studies of Nanosilver molecules and Ag-PMMA nanocomposites by DFT calculations have been performed using Gaussian 09 program with GUI (Graphical User Interface), called Gauss view 5.08. The characterization of programs are such as, optimized geometrical parameters, vibrational frequencies, total energy, dipole moments, frontier orbital energies [HOMO and LUMO], energy gaps etc. From the results, it is found that the values of energy gaps decrease with increasing additives ratio, and are in agreement with experimental results. Also, the theoretical properties of all spectral properties (UV-VIS & FTIR) of nanosilver and nanocomposites results are in good agreement with the experimental results.

KEYWORDS: Silver Nano Particles, Nano Composites & Gaussian 09 Program