The physical and chemical properties of metal clusters depend on the atomic structure, determining the lowest-energy structures of clusters is an important step in understanding and utilizing their properties. In this work we use The Density functional theory (DFT) at the generalized gradient approximation level Becke’s three-parameter and the gradient corrected functional of Lee, Yang and Puar (B3LYP) in combination with the basis set LANL2DZ (the effective core potentials and associated double-zeta valence) to determine some of the structural, electronic and vibrational properties of the planar silver clusters as the Raman Activity, the binding energy, the fragmentation energy, the second energy besides the Higher Occupied Molecular orbital (HOMO) and Lower Unoccupied Molecular Orbital (LUMO) in order to calculate the theoretical band gap of flat geometries of silver clusters in the size range (Ag\(_n\) Clusters < 24); In addition an experimental procedure was made to obtain silver nanoparticles in synthetic zeolite A4, it was possible synthesized by using the ion exchange method with some precursors like silver nitrate (AgNO\(_3\)) and synthetic zeolite A4; The silver NP in Zeolite powder were place in oven under thermal treatment at 450 celsius to release the remain water or humidity on it. The main propose was in this work is to match the theoretical values with the experimental samples synthesized. Transmission Electron microscopy was used to determine the morphology of the particles.

Keywords: Clusters, Nanoparticles, Density Functional Theory

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