Density functional theory (DFT) at the level B3LYP and the basis set LANL2DZ , at ground state energy have been utilized with sophisticated algorithms in Gaussian 09 to investigate molecular geometries, contour density maps, electrostatic potentials (ESPs), infrared spectra (IR), electronic states HOMO and LUMO energies, Energy gaps (E_g), ionization potential (I.P), electron affinity (E.A),dipole moment, polarizabilities, symmetry and density of states of (Au_{10}-OTS) , (Au_{15}) , (Au_{15}-OTS) , (Au_{18}) , (Au_{18}-OTS) , (Ag_{10}) , (Ag_{10}-OTS) , (Ag_{15}) , (Ag_{15}-OTS) , (Ag_{18}) , (Ag_{18}-OTS) , (Cu_9) , (Cu_9-OTS) , (Cu_9-Pyrimidine) and (Cu_{10}). Calculations of (DFT) for (Au_{10}) and (Cu_{10}-Pyrimidine) have been achieved at the level B3LYP and the basis set LANL2MB. However, calculations (DFT) for (Cu_{10}-OTS) has been accomlished at the level B3LYP and the basis set 6-31G.

Physisorption and charge transfer impact apparently to the geometrical nanostructure and electrostatic potentials. Distortion in contour density maps at transition nanometal surfaces because of physisorption and for the atoms of organic nanomaterials as a result to charge transfer. So IR schematics shows that physisortion at the surfaces of the transition nanometal and charge transfer from transition nanometal to organic nanomaterial lead to new active groups as a result to the interaction between the organic nanomaterials and transition nanometal. Gold, silver and copper surfaces demonstrate as semiconductors as compared with original properties, this enable to utilize them in semiconductor technologies in different fields. (Cu_9) has the best value of ionization potential (4.09 eV), but (Au_{10}) stands for the best acceptor. Dipole moment, polarizabilities ant symmetry influenced clearly by physisorption phenomena and charge transfer mechanism. Some nanostructures acquire anti-ferromagnetic properties, but in other nanostructures anti-ferromagnetic feature disappear as a result to physisorption phenomena and charge transfer mechanism.