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Quantum mechanical investigation of CO, NO and HCN adsorption on Ag8 nanoclusters; (structural, electronic and topological properties) HADI AKBARZADEH, ZAHRA TORBATIAN, S. JAVAD HASHEMIFAR, Isfahan University of Technology — We used DFT-GW method to study pure Ag8 nanocluster and CO, NO, HCN adsorption on it. The pure Ag8 stabilizes in Td structure and the behavior of binding energy is consistent with the total charge density at bond points while bond length exhibits a behavior similar to the mean bond charge. Adsorption of CO, NO and HCN molecules on different atomic sites of Ag8 were studied and it was found that all these molecules, mainly due to electron donation, prefer to be adsorbed by LUMO orbital. This finding is in qualitative agreement with the experimental observation of the enhanced binding of CO molecule on positively charged silver atoms, compared with the neutral and negatively charged samples [J. Phys. Chem. A 2006, 110, 7167-7172]. Our calculation shows no significant charge transfer during NO adsorption on Ag8. The CO, NO and HCN adsorbed nanoclusters as well as cationic and anionic samples do not stabilize in Td structure. This charge induced geometry transition is related to the high (low) value of LUMO (HOMO) state in Td structure which indicates high energy cost of electron donation (acceptation) in this isomer. The topological analysis of electron density clarify that the adsorption energy of molecules on Ag8 is consistent with the value of the charge density at the topological bond point between molecule and nanocluster.

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