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On the electronic and structural properties of thiolate protected gold nano-particles $Au_{25-x}Ag_x(SCH_3)_{18}$ **(For x = 6,7,8)** GIHAN PANAPITIYA, West Virginia Univ, HONG WANG, hong.wang@mail.wvu.edu , JAMES P. LEWIS, West Virginia Univ — Thiolate protected gold nanoparticles are among the highly studied nano-structures due to their extraordinary stability and possible applications in catalysis, bio-labeling, chemical sensing and molecular electronics. Doping these nanoparticles with a second metal like Ag have been found to alter optical absorption and chemical properties. In this study, we explore the structural, electronic and chemical properties of a bi-metalic nanoparticle of the form $Au_{25-x}Ag_x(SCH_3)_{18}$ (For x = 6,7,8). Due to the enormity of the number of different doped structures, we choose 500 random configurations for each doping level and energetically optimize them using DFT methods as implemented in Fireball. The lowest energy structures selected thereby are used to study the density of states and to determine the most favorable Ag doping sites. We also calculate the Fukui functions to analyze the chemical selectiveness of different sites of these structures to reactants used in catalytic processes.

Gihan Panapitiya
West Virginia Univ

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