

عنوان مقاله:

Interaction of Amino Acids with Gold and Silver Clusters

محل انتشار:

دومین کنگره بین المللی علوم و فناوری نانو (سال: 1387)

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نویسندگان:

A.H Pakiari - Department of Chemistry , College of Sciences, Shiraz University, Shiraz ۷۱۴۵۴, Iran

Z Jamshidi

خلاصه مقاله:

Gold nanoparticles have attracted much attention in chemistry and material science because of their good biocompatibility, facile synthesis, and conjugation to a variety of bimolecular ligands, antibodies, and other targeting moieties, which make them suitable for the use in biochemical sensing and detection [1-3]. Detection of amino acids is very important in proteomics. One of the major difficulties associated with the selective detection of α -amino acids and peptides using chemosensors is their structural similarity, incorporating both carboxylic and amino groups. Among various amino acids, the S-containing cysteine and cystine amino acids are the most interesting because, being often on the border of large proteins, they provide a link to anchor proteins to metal compounds containing gold and silver. K. G. Thomas et al [4] have reported a novel strategy for the selective detection of micromolar concentrations of cysteine and glutathione by exploiting the interplasmon coupling in Au nanorods. They claimed that they can selectively detect micromolar concentration of cysteine/glutathione from a pool of α -amino acids. Here we have investigated theoretically the interaction of amino acids with Au₃ and Ag₃ clusters which serve as simple catalytic models of Au and Ag nanoparticles. The chosen amino acids are glycine and cysteine in three different forms (cationic)(+, anionic(and neutral()). Atoms-in-Molecules (AIM) theory was applied to determine the nature of bonds between the amino acids and clusters. Natural Bond Orbital (NBO) analysis was also performed to calculate the charge transfer, Wiberg bond indices and natural population analysis (NPA) of the complexes

کلمات کلیدی:

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