Ab initio pseudopotential study of cluster growth of coinage metal telluride clusters Au_nTe_m

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Abstract. The geometries of the lowest-lying isomers of small Au_nTe_m (n, m=1, 2) clusters are determined through the MP2 method. The aspect of gold-telluride interaction, the electron correlation and relativistic effects on geometry, and cluster growth are investigated at the MP2 and CCSD(T) theoretical levels. The results show that the gold-telluride interaction is strong enough to modify the known pattern of bare gold clusters. The electron correlation and relativistic effects are responsible not only for gold-gold attraction but also for additional gold-telluride interaction. Both electron correlation and relativistic effects are essential for determining the geometry and cluster growth of coinage metal telluride compound clusters Au_nTe_m.

1 Introduction

The study of coinage metal mixed clusters, especially the clusters consist of coinage metals mixed with 16 group atoms, is nowadays an important field of research in cluster science since the clusters are widely used in protein, catalysis, microelectronics and so on [1]. The relevant physical and chemical properties, greatly determined by the cluster size, represent great advantages compared to other molecular systems as far as nanostructured materials technology is concerned. The unique characters of this type of clusters are the dramatic effect of gold-mixed atom interaction, electron correlation and relativistic effects that directly influence the structure, stability and cluster growth.

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There exists a considerable amount of theoretical studies on different properties of clusters consisting of coinage metals mixed with 16 group atoms [2–4]. Recently, the structural properties of small clusters Au_nS (n=1-5) and Au_nS_2 (n=1-4), and the aspect of gold-sulphur interaction and its effects on the most stable geometries of the clusters, have been studied by Bravo-Prez *et al*. [5]. In Refs. [6–12], we investigated the small coinage metal telluride clusters $(M_2Te)_n$ (M=Cu, Ag, Au; n=1, 2, 3) and M_nPo (M=Cu, Ag, Au; n=1, 2) systems, and found out that the electron correlation has a strong influence on the bond angle of the clusters but does not change the bond length significantly. The relativistic effects lead to shorter M-Te bond length, lower energies, and increased vibrational frequencies. However, the cluster growth of coinage metal telluride clusters Au_nTe_m, especially the aspect of gold-telluride interaction, electron correlation and relativistic effects on cluster growth have not been studied systematically both by experiment and theoretical approaches.

In this paper, we investigate the aspect of cluster growth and structural properties of coinage metal telluride clusters Au_nTe_m up to n, m = 1, 2. From the calculation, we not only achieve an insight into the energetic of the various isomers that have not been measured experimentally, but also gain characteristics of the gold-telluride interaction, electron correlation and relativistic effects on cluster growth. As the calculated results are in good agreement with our previous results [2–12], we expect that these values are reasonable estimates, even though no experimental data are available at present.

In Section 2, we briefly describe our theoretical approach. Results for investigation are given in Section 3. Section 4 contains a summary of our results.

2   Computational details

The Møller-Plesset second order perturbation theory method (MP2) was used to determine the total energy of the lowest-lying isomers of the clusters. For the Au atom, the relativistic effective small-core pseudopotential (LANL2DZ) and the basis sets of Hay and Wadt (HW) [13] have been used. Under this approximation, the $5d^{10}6s$ outermost valence electrons of the Au atoms are described through a double-zeta (DZ) basis set $(3s3p3d)/[2s2p2d]$. The p exponents of the basis set were optimized considering the best agreement with the experimental spectroscopic values of the Au_2 dimer [14]. For the Te atom, an ECP and DZ basis set given by Hay and Wadt [15] has been used taking the $3s^23p^4$ as valence electrons, and one d function was also included with an optimized exponent.

The electron correlation effects are investigated at the Møller-Plesset second order perturbation theory method (MP2) and the coupled cluster formalism restricted to single and double excitation augmented by a perturbational estimate for triple excitation (CCSD(T)) theoretical levels employing the above mentioned pseudopotential and basis sets (HW) [13–15]. In order to elucidate the role of relativistic effects on structure and stability, we carried out further relativistic and nonrelativistic calculations on the most