



سمینار هفتگی ماده چگال نرم

Theoretical Investigation on the Nature of Interacting Coinage Metal Nano-Clusters with Amino Acids and Chalcogen

Nazanin Jamshidi

School of Chemistry
University of Tehran

In the first part of this lecture, interaction of gold and silver clusters with amino acids (Glycine and Cysteine) is studied using density functional theory (B3LYP). This work demonstrates that the interaction of amino acids with gold and silver cluster is governed by two major bonding factors: a) The anchoring N–Au(Ag), O–Au(Ag) and S–Au(Ag) bonds, and b) The non-conventional N–H...Au(Ag) and O–H...Au(Ag) hydrogen bonds. Among the three forms of amino acids, (anionic, cationic and neutral) anionic ones exhibited the most tendency to interact with the Au and Ag clusters.

In the second part of this lecture, interaction of chalcogen dihydrides (H_2E ; E = O, S, and Se) with small coinage metal clusters like (M_n ; M = Cu, Ag, and Au, n= 3 and 4) is studied by means of density functional theory, with a focus on the nature of chalcogen-metal bonds. For these three metals, binding energy calculations indicate that gold has the highest and silver has the lowest affinities for interaction with H_2E . It is found that interaction of H_2E molecules with the coinage metals increases in order of $H_2Se > H_2S > H_2O$. The nature of M-E bonds is also interpreted by means of the quantum theory of atoms in molecules (QTAIM) and natural bond orbital (NBO) analyses. Natural resonance theory (NRT) is used to calculate natural bond order and bond polarity.

زمان: شنبه ۸۸/۱۲/۱۵ ، ساعت : ۱۵:۳۰

مکان: آمفی تئاتر دانشکده فیزیک