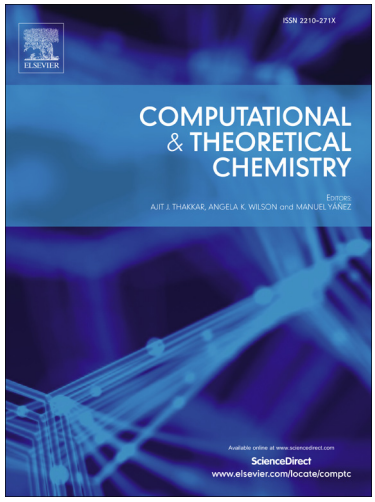

Density functional theory study of the structures and electronic properties of copper and sulfur doped copper clusters

Cheng-Gang Li, Yu-Quan Yuan, Yan-Fei Hu, Jie Zhang, Ya-Nan Tang, Bao-Zeng Ren

PII: S2210-271X(16)30002-0
DOI: http://dx.doi.org/10.1016/j.comptc.2016.01.018
Reference: COMPTC 2046

To appear in: *Computational & Theoretical Chemistry*

Received Date: 30 November 2015
Revised Date: 27 January 2016
Accepted Date: 27 January 2016

Please cite this article as: C-G. Li, Y-Q. Yuan, Y-F. Hu, J. Zhang, Y-N. Tang, B-Z. Ren, Density functional theory study of the structures and electronic properties of copper and sulfur doped copper clusters, *Computational & Theoretical Chemistry* (2016), doi: http://dx.doi.org/10.1016/j.comptc.2016.01.018

Density functional theory study of the structures and electronic properties of copper and sulfur doped copper clusters

Cheng-Gang Li [a, b], Yu-Quan Yuan [c *], Yan-Fei Hu [c], Jie Zhang [a], Ya-Nan Tang [a], Bao-Zeng Ren [b]

[a] *College of Physics and Electronic Engineering, Quantum Materials Research Center, Zhengzhou Normal University, Zhengzhou 450044, China*

[b] *School of Chemical Engineering and Energy, Zhengzhou University, Zhengzhou 450001, China*

[c] *School of Science, Sichuan University of Science & Engineering, Zigong 643000, China*

Abstract:

The structures and electronic properties of copper and sulfur doped copper clusters have been systematically investigated by means of the CALYPSO structure searching method combined with density functional theory. According to optimized Cu_nS geometries, the dominant growth pattern is described as one Cu atom being added on the $Cu_{n-1}S$ clusters. The planar (C_{2v}) Cu_2S cluster is the most stable geometries of Cu_nS clusters. From n=3, the doped systems show the appearance of three-dimensional (3*D*) geometries. In addition, the calculated HOMO-LUMO gaps are in the energy range of 1.42-2.96 eV, which make Cu_nS clusters suitable candidates for renewable energy sources. At last, the molecular orbital energy, density of states, electrostatic potential and electron density deformation are also respectively analyzed for realizing the doped microscopic mechanism and providing strong support for essential theoretical and experimental research.

Keywords: CALYPSO; Density functional theory; Cu-S cluster

1. Introduction

It is well known that the energy sources are a serious problem in current society. Looking for a

*Correspondence to: Yu-Quan Yuan, School of Science, Sichuan University of Science & Engineering, Zigong 643000, China.
E-mail address: yuquan_yuan1975@suse.edu.cn