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2008 J. Phys.: Condens. Matter 20 064214

(http://iopscience.iop.org/0953-8984/20/6/064214)

J. Phys.: Condens. Matter **20** (2008) 064214 (1p) doi:10.1088/0953-8984/20/6/064214

Elucidation of the Au–S bond in a passivated gold cluster through density functional theory calculations

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Received 17 December 2007
Published 24 January 2008
Online at stacks.iop.org/JPhysCM/20/064214

Abstract

Gold clusters are of increasing interest due to a number of already established as well as new potential applications in different fields of nanotechnology. The use of gold nanoparticles can be significantly extended by surface modifications, sulfidation being the most popular. The identifications of preferred adsorption geometries, bond formation, and binding energies are helpful tools for understanding the properties of these particles.

This study is focused on a 38-atom gold cluster passivated with 3-hydroxypropanthiolate linkers. Starting from the re-optimized global minimum structure of a bare 38-atom gold cluster (Doye and Wales 1998 *New J. Chem.* **22** 733–44) and aiming at a description of the passivated particle, density functional theory calculations (within the framework of the Amsterdam density functional calculation package ADF 2006.01 (ADF2006.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com)) were performed at the level of the generalized gradient approximation of Perdew and Wang from 1991, with triple-zeta Slater basis sets plus p- and f-polarization functions (TZ2P) for the 33 outermost electrons of each gold atom, and considering scalar relativistic effects. Using this methodology, the space around the gold cluster (with the distance of the S of the thiolate from the gold cluster surface in the range 2.3–2.6 Å) was examined to identify the most favourable absorption site for the thiolate linker. As a result, a 3D map was created and low energy areas corresponding to the potentially most favourable site for one 3-hydroxypropanthiolate linker on the gold cluster localized. Structures representing these areas were further optimized and consequently analysed using Mulliken population analysis to compare charge distribution over the tested structures, Mayer bond order analysis, as well as electron localization function/indicator bond formation analysis.

The results obtained will be presented in comparison to ones available from studies of other research groups.

