

Theoretical exploration of seleno and tellurophenols as promising alternatives to sulfur ligands for anchoring to gold (111) materials

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RSC ADVANCES

Volumen: 6

Número: 6

Páginas: 4458-4468

DOI: 10.1039/c5ra21964g

Fecha de publicación: 2016

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Resumen

It is widely known that sulfur ligands, such as alkanethiols or phenothiols and their derivatives, are useful anchor systems for gold materials due to the high affinity of sulfur to gold surfaces. In this study we use DFT calculations and a 42-atom gold cluster model to study the interaction between selenophenol and tellurophenol-derivatives with the Au(111) surface to gain information towards potential new gold-based materials. We modulated the interaction strength by controlling the charge transfer process of a particular interaction by chemically modifying the ligands. To obtain a complete analysis, we studied the ligands in their protonated, anionic and radical states aiming to cover the three possibilities in which these may interact with the gold cluster. In order to get a deeper insight into the nature of the interaction we used several analysis techniques such as energy decomposition analysis (EDA), non-covalent interactions (NCI) and natural population analysis (NPA). Our results reveal that tellurium in the anionic state provides complexes of better thermodynamic stability by similar to 12.0 kcal mol, when compared with the strongest sulfur-gold complex, also in the anionic state. Furthermore, this indicates that the anionic ligand is probably the dominant state for both selenium and tellurium as observed previously for sulfur. The extent to which the interaction strength could be controlled directly depends on the state of the anchor atom. In our case the anionic state is the most suitable for tuning the interaction. Finally, our main findings suggest that exchanging sulfur with selenium or tellurium involves an important increase of the interaction strength, thus, making these selenophenol and tellurophenol derivatives attractive for the development of new functional materials.

Palabras clave

KeyWords Plus: SELF-ASSEMBLED MONOLAYERS; CHELATING DIARYLOXO LIGANDS; TITANIUM COMPLEXES; FORCE MICROSCOPY; CHARGE-TRANSFER; CHAIN-LENGTH; BASIS-SETS; CHEMISTRY; SURFACES; PSEUDOPOTENTIALS

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Financiación

Entidad financiadora	Número de concesión
FONDECYT	3130383 1140503 1150629
Grant ICM	120082
CONICYT	21130874
German Research Foundation (DFG)	EXC 310/2

[Ver texto de financiación](#)

Editorial

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Categorías / Clasificación

Áreas de investigación:Chemistry

Categorías de Web of Science:Chemistry, Multidisciplinary

Información del documento

Tipo de documento:Article

Idioma:English

Número de acceso: [WOS:000369510500023](#)

ISSN: 2046-2069

Información de la revista

- Impact Factor: [Journal Citation Reports®](#)

Otra información

Número IDS: DC8ZT

Referencias citadas en la Colección principal de Web of Science: **52**

Veces citado en la Colección principal de Web of Science: **0**