Au13-nAgn clusters: a remarkably simple trend

Por: Munoz, F (Munoz, Francisco)[1,2] ; Varas, A (Varas, Alejandro)[1,2,3,4] ; Rogan, J (Rogan, Jose)[1,2] ; Valdivia, JA (Alejandro Valdivia, Juan)[1,2] ; Kiwi, M (Kiwi, Miguel)[1,2]

PHYSICAL CHEMISTRY CHEMICAL PHYSICS
Volumen: 17
Número: 45
Páginas: 30492-30498
DOI: 10.1039/c5cp05664k
Fecha de publicación: 2015
Ver información de revista

Resumen

The planar to three dimensional transition of Au13-nAgn clusters is investigated. To do so the low lying energy configurations for all possible concentrations (n values) are evaluated. Many thousands of possible conformations are examined. They are generated using the procedure developed by Rogan et al. in combination with the semi-empirical Gupta potential. A large fraction of these (the low lying energy ones) are minimized by means of Density Functional Theory (DFT) calculations. We employ the Tao, Perdew, Staroverov, and Scuseria (TPSS) meta-GGA functional and the Perdew, Burke and Ernzerhof (PBE) GGA functional, and compare their results. The effect of spin-orbit coupling is studied as well as the s-d hybridization. As usual in this context the results are functional-dependent. However, both functionals lead to agreement as far as trends are concerned, yielding just two relevant motifs, but their results differ quantitatively.

Palabras clave

KeyWords Plus:TOTAL-ENERGY CALCULATIONS; LENNARD-JONES CLUSTERS; WAVE BASIS-SET; GOLD CLUSTERS;GLOBAL OPTIMIZATION; ELECTRONIC-PROPERTIES; SIZE; TRANSITION; SURFACE; PERFORMANCE

Información del autor

Dirección para petición de copias: Kiwi, M (autor para petición de copias)

+ Univ Chile, Fac Ciencias, Dept Fis, Casilla 653, Santiago 7800024, Chile.

Direcciones:

+ [1] Univ Chile, Fac Ciencias, Dept Fis, Santiago 7800024, Chile

[2] Ctr Desarrollo Nanociencia & Nanotecnol CEDENNA, Santiago 9170124, Chile

+ [3] Univ Pais Vasco UPV EHU, Nanobio Spect Grp, E-20018 San Sebastian, Spain

+ [4] Univ Pais Vasco UPV EHU, ETSF Sci Dev Ctr, Dept Fis Mat, E-20018 San Sebastian, Spain

Direcciones de correo electrónico:m.kiwi.t@gmail.com

Financiación

Entidad financiadora	Número de concesión
Fondo Nacional de Investigaciones Cientficas y Tecnologicas (FONDECYT, Chile)	11110510 1150806 1150718 1120399 1130272
Financiamiento Basal para Centros Cientficos y Tecnologicos de Excelencia	FB0807

Ver texto de financiación

Editorial

ROYAL SOC CHEMISTRY, THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS, ENGLAND

Categorías / Clasificación

Áreas de investigación: Chemistry; Physics

Categorías de Web of Science: Chemistry, Physical; Physics, Atomic, Molecular & Chemical

Información del documento

Tipo de documento: Article

Idioma: English

Número de acceso: WOS:000364862000030

ID de PubMed: 26513198

ISSN: 1463-9076

eISSN: 1463-9084

Información de la revista

- **Impact Factor:** Journal Citation Reports®

Otra información

Número IDS: CW2ZP

Referencias citadas en la Colección principal de Web of Science: 41

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