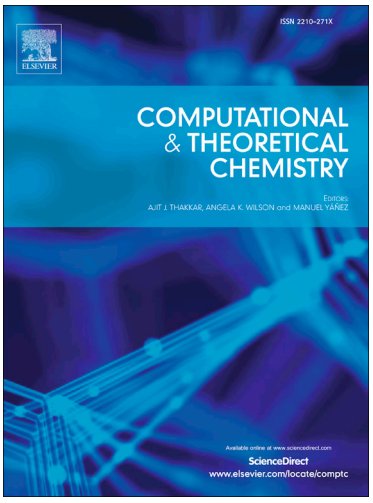


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PII: S2210-271X(18)30115-4
DOI: https://doi.org/10.1016/j.comptc.2018.03.033
Reference: COMPTC 2767

To appear in: *Computational & Theoretical Chemistry*

Received Date: 22 February 2018
Revised Date: 30 March 2018
Accepted Date: 30 March 2018

Please cite this article as: S. Zhao, Y. Ren, K. Yao, X. Tian, J. Wang, J. Liu, Stability, structural and electronic properties of ternary $Pd_x Au_y Ag_z$ clusters ($x$+$y$+$z$=7): A theoretical study, *Computational & Theoretical Chemistry* (2018), doi: https://doi.org/10.1016/j.comptc.2018.03.033

# Stability, structural and electronic properties of ternary $Pd_xAu_yAg_z$ clusters ($x$+$y$+$z$=7): A theoretical study

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**ABSTRACT** Full range of Au and Ag doped Pd clusters, $Pd_xAu_yAg_z$ with $x$+$y$+$z$=7 in their ground states, are studied using the density functional theory (DFT) at TPSSTPSS method with SDD pseudopotential. The average interatomic distance, chemical order, charge distribution, binding energy, mixing energy, finite difference energy, vertical ionization potential, electron affinity and HOMO-LUMO gap of the ternary clusters are evaluated as a function of the whole concentration range, from which the mutual influences of Au and Ag dopants on the properties of Pd cluster are predicted and analyzed.

**Keywords:** Density functional theory; Ternary clusters; Electronic properties

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