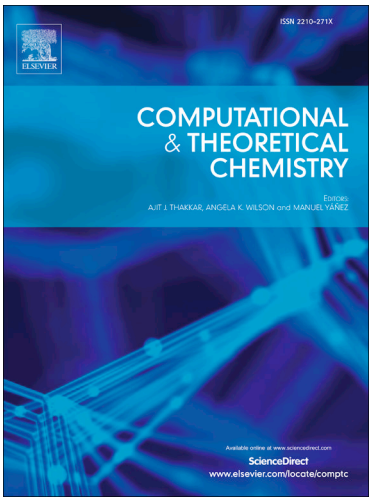

Structural, electronic and catalytic properties of single magnesium atom doped small neutral Rh_n (n=2-8) clusters: Density functional study

Abhijit Dutta, Paritosh Mondal

PII: S2210-271X(17)30322-5
DOI: http://dx.doi.org/10.1016/j.comptc.2017.07.003
Reference: COMPTC 2565

To appear in: *Computational & Theoretical Chemistry*

Received Date: 4 October 2016
Revised Date: 16 June 2017
Accepted Date: 3 July 2017

Please cite this article as: A. Dutta, P. Mondal, Structural, electronic and catalytic properties of single magnesium atom doped small neutral Rh_n (n=2-8) clusters: Density functional study, *Computational & Theoretical Chemistry* (2017), doi: http://dx.doi.org/10.1016/j.comptc.2017.07.003

Structural, electronic and catalytic properties of single magnesium atom doped small neutral Rh_n (n=2-8) clusters: Density functional study

Abhijit Dutta, Paritosh Mondal*

Department of Chemistry, Assam University, Silchar 788011, Assam, India

*Corresponding author: Email: paritos_au@yahoo.co.in

Abstract

Rhodium nano clusters exhibit unique electronic, magnetic and catalytic properties. Physical and chemical properties of rhodium cluster can be tuned by incorporating different metal and non metal atoms. In this study magnesium doped rhodium clusters are investigated to evaluate their structure, stability, electronic and magnetic properties using density functional theory (DFT). Stability function, fragmentation energy and LUMO-HOMO gap reveals that Rh_5Mg, Rh_6Mg and Rh_8Mg clusters are more stable than the other magnesium doped rhodium clusters. Chemical reactivity of rhodium cluster increases on doping with magnesium atom. Deformation density, density of electronic state, force vector analysis suggest that electronic redistribution are occurred to attain the higher stability in Rh_5Mg as well as in Rh_8Mg. Negative electrostatic potential is generally generated on rhodium atoms opposite to magnesium atom while, electrons are transferred from magnesium to rhodium atoms in magnesium doped rhodium clusters. Calculated structural, electronic and orbital parameters suggest higher stability of Rh_5Mg, Rh_6Mg and Rh_8Mg clusters. Magnesium doped rhodium clusters are found to be more reactive than pure rhodium clusters on the basis of evaluated Fukui function values. Rh_5Mg cluster is seen to be better catalyst for the dissociation of CH_3OH in comparison to pure Rh_5. Activation of O−H bond is observed to be more favourable in comparison to methyl C−H bond in the dissociation of CH_3OH.

Key words: Rhodium, Magnesium, DFT, stability, force vector, CH_3OH.