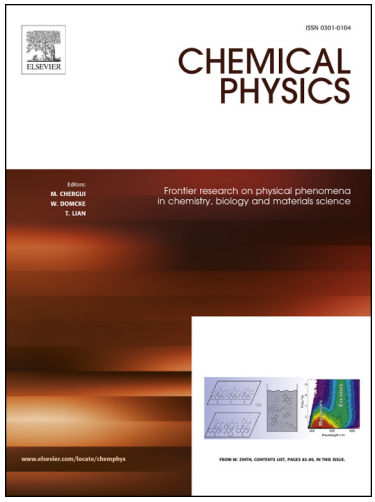

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PII: S0301-0104(14)00195-5
DOI: http://dx.doi.org/10.1016/j.chemphys.2014.07.004
Reference: CHEMPH 9139

To appear in: *Chemical Physics*

Received Date: 20 November 2013
Accepted Date: 3 July 2014

Please cite this article as: B. Hamad, Z. El-Bayyari, A. Marashdeh, Investigation of the stability of platinum clusters and the adsorption of nitrogen monoxide: first principles calculations, *Chemical Physics* (2014), doi: http://dx.doi.org/10.1016/j.chemphys.2014.07.004

Investigation of the stability of platinum clusters and the adsorption of nitrogen monoxide: first principles calculations

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Abstract

Density Functional Theory (DFT) calculations are performed to investigate the structural, energetic, electronic and magnetic properties of bare Pt_n (n = 2-6. 8, 10, 13, 30 and 39) isomers. Our calculations show that small sized Pt configurations prefer to form planar structures, while for larger size clusters, the structures tend to be compact. The most stable isomers have been selected to study the adsorption of nitrogen monoxide molecule (NO) on them. Our results show that the most stable adsorption sites of NO on Pt clusters are the top site for Pt with n=2-4, while the bridge site is favorable for the rest of the clusters (Pt with n=5, 6, 39). Our findings show that the bridge site of large clusters softens the NO bond more than the top site of smaller clusters.

Keywords: DFT, Pt clusters, NO, Adsorption

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I. Introduction

It has been extensively proved that the miniaturization and descending of the size of materials to the nanoscale region lead to properties much different than those of the bulk due to the quantum size effect. Such nanostructured materials exhibit very interesting physical and chemical properties, which are playing a vital role in enhancing