### Accepted Manuscript

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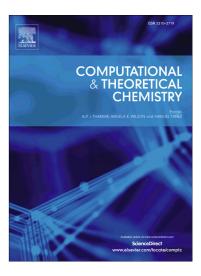
PII: S2210-271X(16)30447-9

DOI: http://dx.doi.org/10.1016/j.comptc.2016.11.008

Reference: COMPTC 2294

To appear in: Computational & Theoretical Chemistry

Received Date: 28 September 2016 Revised Date: 6 November 2016 Accepted Date: 7 November 2016



Please cite this article as: K.O. Alcantar-Medina, M. Herrera-Trejo, A. Tlahuice-Flores, S. Martinez-Vargas, J. Oliva, A.I. Martinez, Evolution of the structural and electronic properties of small alkali metal-doped aluminum clusters, *Computational & Theoretical Chemistry* (2016), doi: http://dx.doi.org/10.1016/j.comptc.2016.11.008

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## **ACCEPTED MANUSCRIPT**

# Evolution of the structural and electronic properties of small alkali metal-doped aluminum clusters

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#### **Abstract**

The atomic arrangement of  $Al_n$  and  $Al_nM$  clusters (n = 2 - 14, M = Li, Na o K) was determined by combining both the basin hopping (BH) algorithm using the Gupta potential, and density functional theory (DFT) calculations. The BH yielded hundreds of structures that were refined by DFT using the PBE framework, and Ahlrichs-VDZ basis sets. Anions, neutrals and cations of  $Al_n$  and  $Al_nM$  clusters were calculated by DFT resulting in a set of ground state structures. These structures were considered for studying different stability criteria such as binding energy,

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