

A DFT study of the structure and stability of Al-Mg nanoclusters

PELUZO, B. M. T. C.*¹, PAIVA, M. A. M.*², GALVÃO, B. R. L.*³

* Departamento de Química, Centro Federal de Educação Tecnológica de Minas Gerais, Belo Horizonte, Brazil

Synopsis Nanoalloys containing aluminium and magnesium up to 30 atoms obtained by an empirical potential were optimized via DFT calculations.

Magnesium and Aluminium are known for lightness, abundance and can be employed in hydrogen storage. When doped, they become even more efficient in hydrogen absorption [1]. Although Al-Mg clusters were previously studied in the literature [1, 2], electronic structures calculations were performed for clusters with less than 15 atoms only. In this work, Al-Mg clusters containing up to 30 atoms have been investigated: an average of 10 structures for each composition, generated by a genetic algorithm, associated with the Gupta empirical potential, were optimized using the package GAMESS-US, B3LYP functional and LANL2DZ basis set with an ECP.

provides a comparison between an alloy and its homonuclear counterparts: negative values mean preference for the mixed compositions. By analysing these plots (Fig. 1), one notes the alloys are favored only for larger clusters.

$$E_{exc} = V_{Al_xMg_{N-x}} - \frac{x}{N}V_{Al_N} - \frac{N-x}{N}V_{Mg_N} \quad (1)$$

Structures obtained after DFT optimizations present more compact geometry and, differently from GA results, not all of them show the preference for Al atoms to stay at the core. Reactivity may be investigated by the gap between HOMO and LUMO orbitals, where high values mean resistance to oxidation [1]. Fig. 2 shows a plot of the gap as a function of the number of valence electrons, where peaks are obtained at 20 and 40, which correspond to closed shell structures in the jellium model. After such calculations, it is possible to conclude that some of the Al-Mg clusters are producible, which may have several applications in nanotechnology, like hydrogen storage and catalysis. Further calculations for structures containing up to 55 atoms are being carried out.

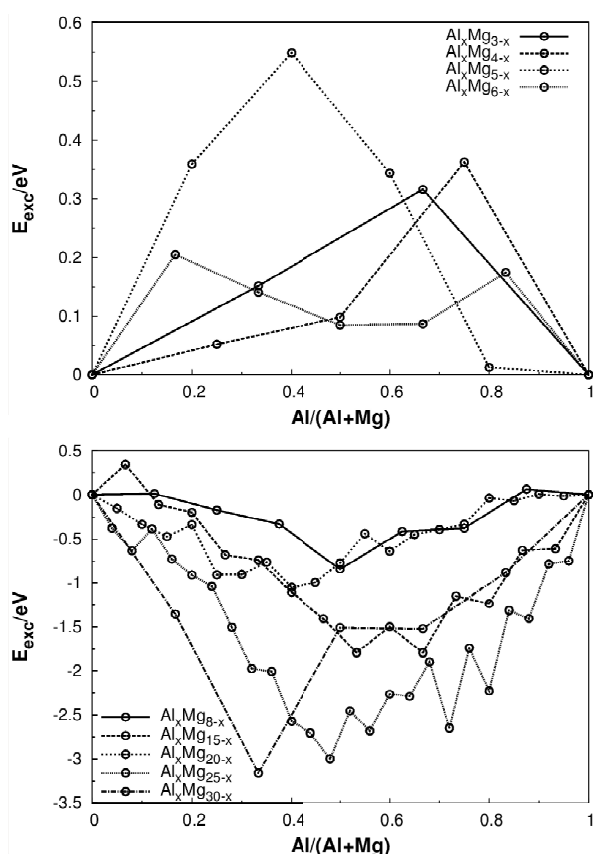


Figure 1. Excess energy plots for 3, 4, 5, 6, 8, 15, 20, 25 and 30 atoms structures.

In order to analyze the obtained results, Eq.1 was used to calculate the excess energy, which

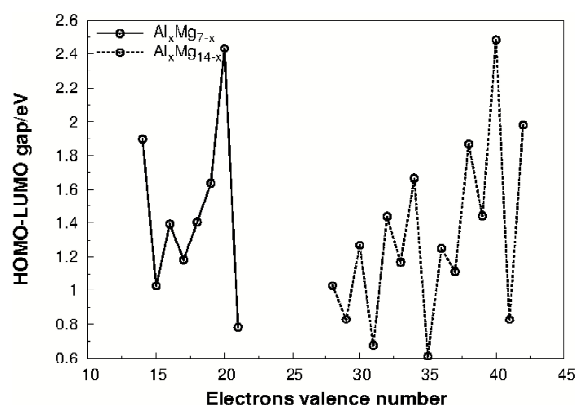


Figure 2. Gap plot for 7 and 14 atoms clusters.

References

- [1] Luo Z. *et al.* 2013 *J. Am. Chem. Soc.* **135** 4307
- [2] Osorio E. *et al.* 2013 *Phys. Chem. Chem. Phys.* **15** 2222

¹E-mail: barbarapeluzo@gmail.com

²E-mail: mts381@gmail.com

³E-mail: brenogalvao@gmail.com