EVOLUTION OF THE PROPERTIES IN Al_nN_n CLUSTERS WITH SIZE.

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The electronic properties of aluminum nitride makes it suitable for the fabrication of light emitting diodes and a new generation of short-wavelength lasers. It also has multiple applications in microelectronic elements for high-temperature and high power devices.Though this material has been studied extensively in solid state and thin film forms, research at the micro-and nanocluster levels is still lacking.

In this contribution, we present a new technique to study the evolution of the properties aluminum nitride from nanostructures to the bulk.We simulate Al_nN_n clusters containing from one molecule (n=1) to one hundred molecules (n=100). The main problem in this study lies in the need for an exhaustive exploration of the geometrical configuration space to locate the lowest energy isomer , that becomes extremely costly computationally when the cluster size increases or when the effective dimensionality of the cluster changes.To perform this exam, we have used our cluster code.[1]. This is an atomistic program that allows to generate thousands of isomers or stable configurations of a given molecular complex by means of a Montecarlo basin hopping global mimization method. We describe the interactions among the different atoms in the cluster by means of a simpleBorn-Mayer like potential.

As results of this study, we present the choice of sizes and the most relevant features of the lowest energy isomers. Subsequently, we show the obtained properties classified in five different categories: energetic, geometric, coordination, electrostatic, and vibrational properties.

References[1] The cluster program. EvelioFrancisco;Universidad de Oviedo,2001-2005.