

Abstract Submitted
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Size-Evolution of the Structural and Energy Characteristics of Magnesium Clusters¹ PAULO H. ACIOLI², JULIUS JELLINEK, Chemistry Division, Argonne National Laboratory, Argonne, IL 60439 — The most fascinating and important from the applied point of view attribute of the cluster phase of matter is the unique and often unexpected variation of properties with the cluster size. The structural forms, electronic properties, nature and strength of bonding, and other physical characteristics all change as the clusters grow. The rate of change in different properties is, however, nonuniform and element/material dependent. The goal of this study is to investigate and characterize qualitatively and quantitatively the size evolution of the structural and energy characteristics of magnesium clusters. These include the transition from a tetrahedral- to pentagonal- to capped trigonal prism-based motif as the energetically most preferred one. The analysis will include also the higher energy isomers of the clusters and will address the issue of the transition to the bulk lattice.

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