

Abstract Submitted
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Heusler clusters¹ ALEXEY ZAYAK, University of Texas at Austin, SCOTT BECKMAN, Rutgers University, MURILO TIAGO, Oak Ridge Natl. Laboratory, PETER ENTEL, University of Duisburg-Essen, JAMES CHELIKOWSKY, University of Texas at Austin — Real space pseudopotential calculations are used in order to investigate the properties of Heusler clusters. Bulk-like clusters with various Ni-Mn-Ga compositions have been examined in the size range from 15 up to 169 atoms. Among these compositions the closest to the stoichiometric Ni₂MnGa are the most stable. These clusters retain tendency for tetragonal distortion, which is inherited from the bulk properties. Although, the surface effects dominate suppressing the tetragonal structure in the smaller clusters, the bigger clusters develop a bulk-like tetragonal distortion. We predict the existence of switchable Ni-Mn-Ga clusters, which might be of great interest for the nano-Magnetic-Shape-Memory technology.

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