Abstract Submitted
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Heusler clusters[1] ALEXEY ZAYAK, MURILO L. TIAGO, SCOTT BECKMAN, JAMES R. CHELIKOWSKY, ICES, University of Texas at Austin — Heusler alloys are known for their bulk properties, for example the magnetic shape-memory Ni_2MnGa [1]. Using first principles simulations, based on the real space pseudopotential method implemented in PARSEC [2], we examine Heusler alloy clusters. Clusters with various Ni-Mn-Ga compositions are examined in the size from 15 up to 113 atoms. Clusters with compositions being the closest to the stoichiometric Ni_2MnGa are the most stable. The geometry of tetrahedral coordination in Heusler structures is energetically favorable. In order to retain this coordination, clusters have to be symmetrically shaped. This implies that even in very small clusters the structure is bulk-like. However, the electronic densities of states do not show Kohn-like anomalies at the Fermi level, that are characteristic for bulk Ni-Mn-Ga alloys. [1] P. Entel, V. D. Buchelnikov, V. V. Khovailo et al. J. Phys. D: Appl. Phys. 39, 865 (2006) [2] http://www.ices.utexas.edu/parsec/

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