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Complex magnetic ordering and spin glass behavior as a driving mechanism of multifunctional properties of Heusler alloys from first principles ANNA GRUENEBOHM, PETER ENTEL, HEIKE C. HERPER, MARKUS E. GRUNER, ALFRED HUCHT, DENIS COMTESSE, Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany, RAYMUNDO ARROYAVE, Department of Mechanical Engineering, Texas A&M University, College Station, Texas 77843, USA — First-principles calculations are used to study the structural, electronic and magnetic properties of (Pd, Pt)-Mn-Ni-(Ga, In, Sn, Sb) alloys which display multifunctional properties like the magnetic shape-memory, magnetocaloric and exchange bias effect. The ab initio calculations give a basic understanding of the underlying physics which is associated with the complex magnetic behavior (also spin glass) arising from competing ferro- and antiferromagnetic interactions with increasing number of Mn excess atoms in the unit cell. This information allows to optimize, for example, the magnetocaloric effect by using the strong influence of compositional changes on the magnetic interactions. Thermodynamic properties can be calculated by using the ab initio magnetic exchange parameters in finite-temperature Monte Carlo simulations. We present guidelines of how to improve the functional properties. For Pt-Ni-Mn-Ga alloys, a shape memory effect with 14% strain can be achieved in an external magnetic field.

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