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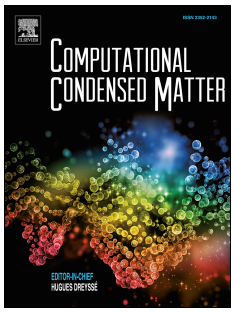

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The First Principle Calculation of Structural, Electronic, Magnetic, Elastic, Thermal and Lattice Dynamical Properties of Fully Compensated Ferrimagnetic Spin-Gapless Heusler Alloy Zr_2MnGa

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Abstract

The first principle calculation for geometry optimization, elastic, electronic, magnetic, thermal, transport and lattice-dynamical properties of new spin gapless full heusler compound Zr_2MnGa were studied within Density Functional Theory approach (DFT). The material obeys Slater Pauling (SP) rule and exhibit spin gapless semiconducting behavior with fully compensated ferrimagnetism (FCF). To the best of our knowledge, various mechanical, thermal, transport and lattice dynamical properties like elastic constant, bulk modulus and Debye temperature are reported for the first time using density functional theory (DFT). The structure satisfies all stability criteria and is thus found stable at equilibrium value of lattice constant. Zr_2MnGa crystallizes in inverse heusler structure which is stable at ground state and have zero magnetic