

Abstract Submitted
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New Class of Mn Based MAX Phases SA LI, PURU JENA, Virginia Commonwealth University, RAJEEV AHUJA, University of Uppsala — The MAX phase materials are a class of ternary compounds with formula unit: $M_{N+1}AX_N$ (MAX), where $N = 1, 2$ or 3 , M is an early transition metal, A is an A-group (mostly IIIA and IVA) element, and X is either C and/or N . These ternary carbides and nitrides combine unusual properties of both the metals and ceramics. They exhibit high hardness, but fully reversible plasticity, and negligible thermoelectric power. In this paper, we report a new series of MAX phases which not only possess the usual properties of the MAX phase, but also are magnetic under ambient conditions. The electronic structure and magnetic properties of Mn based MAX phases have been systematically studied by means of first principles method based on the density functional theory. By comparing the energy difference between the ferromagnetic and antiferromagnetic configurations for the Mn based MAX phases, we determined that there are one $Mn_2(Al, Si)X$ phase, two $Mn_3(Al, Si)X_2$ phases, and three $Mn_4(Al, Si)X_3$ phases which can be stabilized in the ferromagnetic state. This finding adds a new property to the MAX phase materials for technological applications.

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