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Development of spin-gapless semiconductivity and half metallicity in Ti_2MnAl by substitutions for Al[1] PAVEL LUKASHEV, University of Northern Iowa, SIMEON GILBERT, South Dakota State University, BRADLEY STATEN, NOAH HURLEY, University of Northern Iowa, RYAN FUGLSBY, PARASHU KHAREL, YUNG HUH, South Dakota State University, SHAH VALLOPPILLY, WENYONG ZHANG, University of Nebraska, Lincoln, K. YANG, Hohai University, DAVID J. SELLMYER, University of Nebraska, Lincoln — In recent years, ever increasing interest in spin-based electronics has resulted in the search for a new class of materials that can provide a high degree of spin polarized electron transport. An ideal candidate would act like insulator for one spin channel and a conductor or semiconductor for the opposite spin channel (e.g., half metal (HM), spin-gapless semiconductor (SGS)). Here, we present the combined computational, theoretical, and experimental study of Ti_2MnAl, a Heusler compound with potential application in the field of spintronics. We show that in the ground state this material is metallic, however it becomes a SGS when 50% of Al is substituted with In (e.g., $Ti_2MnAl_{0.5}In_{0.5}$), and a HM when 50% of Al is substituted with Sn (e.g., $Ti_2MnAl_{0.5}Sn_{0.5}$). Detailed study of the structural, electronic, and magnetic properties of these materials is presented.

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Pavel Lukashev
University of Northern Iowa

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