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The Magnetism of $Mn_{2-x}Fe_xB$ Alloys : First-Principles Calculations PO-HAN LEE, Affiliated Senior High School of National Taiwan Normal University, Taipei, Taiwan, SHIH-WEI WANG , Stevenson School, Pebble Beach, CA USA, CHAO-YANG LIN, Department of Electrical Engineering, National Tsing Hua University, Hsinchu, Taiwan, KUAN-LING CHEN, Department of Electrical and Computer Engineering, Cornell University, NY USA, HSUAN-AN HSIA, Affiliated Senior High School of National Taiwan Normal University, Taipei, Taiwan, KUAN-YU CHEN, Department of Physics, National Taiwan University, Taipei, Taiwan , PANG-YU LIU, Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan, KE-BENG CHEN, Department of Law, National Taiwan University, Taipei, Taiwan, EN-HUI LIU, Center for Nanotechnology, Materials Science and Microsystems, National Tsing Hua University, Hsinchu, Taiwan — Magnetic, electronic and structural properties of $Mn_{2-x}Fe_xB$ ($0 \leq x \leq 2$) are investigated by the First principles calculations with the virtual crystal approximation (VCA) based on the density-functional theory (DFT) with generalized gradient approximation (GGA). Although both of Mn_2B and Fe_2B have the same electronic structure of I4/MCM with different lattice constants, the former is anti-ferromagnetic and the latter ferromagnetic. All calculations, based on the four types of magnetic states of NM (non-magnetic), FM (ferromagnetic), AFM1 and AFM2 (anti-ferromagnetic), illustrate that there is a critical point of magnetic phase transition occurred at x as 0.5 from AFM2 to FM state under the condition of the lowest energy. Results are also in agreement with the Stoner model within the range of FM state.

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