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Heusler Alloys for CPP-GMR C. CULBERT, MINT Center, University of Alabama, Tuscaloosa, AL, M. WILLIAMS, Department of Mathematics and Computer Sciences, University of Maryland Eastern Shore, Princess Anne, MD, M. CHSHIEV, P. LECLAIR, W. H. BUTLER, MINT Center, University of Alabama, Tuscaloosa, AL — Half-Metallic full Heusler alloys of composition X_2YZ and structure type $L2_1$ have aroused interest because of their potential application in CPP-GMR spin valves for readers in hard disk drives. The X and Y are typically transition metals and the Z is a non-transition metal element. The structure of these alloys can be viewed as a variant of bcc in which (100) atomic layers of X alternate with layers of YZ. The alloys Co_2MnSi and Co_2MnGe have received particular attention because of their high T_C which exceeds 900K. We have performed first-principles calculations using the VASP code in GGA to investigate the properties of these materials. We have found them to be half-metals in bulk in agreement with previous work. We obtained minority gaps at the Fermi energy of 0.36 and 0.51eV for Co_2MnGe and Co_2MnSi, respectively. We also investigated multilayers consisting of Heusler and various possible spacer materials. Interestingly, we found that for one or two atomic layers of Cr alternating with Co2MnGe along (100), the system remained half-metallic. Cr can actually be used in this way to increase the minority gap. We found that Co_2MnGe slabs were typically not half metallic, but slabs terminated in a pure Mn layer retained a minority gap.

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