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Effects of pressure and strain on spin polarization of IrMnSb PAVEL LUKASHEV, IBRICA TUTIC, JULIANA HERRAN, University of Northern Iowa, BRADLEY STATEN, Pennsylvania State University, PAUL GRAY, University of Northern Iowa, TULA PAUDEL, ANDREI SOKOLOV, EVGENY TSYMBAL, University of Nebraska - Lincoln — A high degree of spin polarization in electron transport is one of the most sought-after properties of a material which can be used in spintronics. An ideal candidate to exhibit highly spin-polarized current would be a room temperature half-metal, a material which behaves as an insulator for one spin channel and as a conductor for the other spin channel. Computational results on structural, magnetic, and electronic properties of a semi-Heusler compound, IrMnSb will be presented. This material has been reported to exhibit pressure induced half-metallic transition. This result is confirmed, and explained by the reduction of the exchange splitting of the spin bands consistent with the Stoner model for itinerant magnetism. It is also shown that the half-metallic transition is suppressed when instead of uniform pressure the bulk IrMnSb is exposed to biaxial strain. This suppression of half-metallicity is driven by the epitaxial strain induced tetragonal distortion, which lifts the degeneracy of the Mn 3d t_{2q} and e_q orbitals and reduces the minority-spin band gap under compressive strain, thus preventing halfmetallic transition. Finally, it is demonstrated that in thin film geometry, surface states emerge in the minority-spin band gap, which has detrimental for practical applications impact on the spin polarization of IrMnSb.

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