Impurity bands and half-metal states in Mn-doped GaS layers
J.T. HARALDSEN, D. PARKER, T. PEKAREK, Univ of North Florida, A.V. BALATSKY, Los Alamos National Laboratory/NORDITA — In this study, we examine the magnetization, electronic band structure, and density of states for Mn doped GaS, which is a quasi-two-dimensional semiconductor. Starting with undoped GaS, we progressively added nine Mn atom into randomly determine Ga sites. We find that as the Mn doping is increased, the magnetization increases linearly with dopant, and the presence of magnetic atoms produces impurity bands in the electronic structure. Furthermore, examination of density of states shows that increase in magnetic impurity bands seems to lead to the presence of a weak, but noticeable, spin polarization at the Fermi level. This leads us to the indication of a possible half-metal state with increased Mn doping or other transition-metal atoms.