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Electronic structure of MS2-LiB under hydrostatic pressure.[1]
EDGAR MARTINEZ-GUERRA, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico., ALEKSEY N. KOLMOGOROV, STEFANO CURTAROLO, Duke Univeristy, North Carolina, USA. — Recently ab initio calculations have found that the Li-B phase equilibrium diagram has two new phases: MS1 and MS2 [A. Kolmogorov and S. Curtarolo, Phys. Rev. B **73**, 180501R (2006)]. These two phases are stable enough to compete against known phases. These lithium borides exhibit electronic features similar to those in magnesium diboride and they are expected to be superconductors. In this work, we have studied the structural and electronic properties of the MS2-LiB system under pressure. The calculations were performed using the SIESTA code, with the GGA exchange-correlation functional in the PBE form. We have used numerical atomic orbitals as the basis set for the valence wavefunctions employing a double ζ-polarized basis. We present a detailed analysis of the band structure, Fermi surface, and orbital populations as a function of the hydrostatic pressure. In particular, we focus on the behavior of the σ- and π-bands derived from the boron p-states.

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