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The Pressure Effect on the Electronic Structure of the Ordered LiBC EBRU GUNGOR, ENGIN OZDAS, Advanced Materials Research Group, Physics Department, Hacettepe University, Beytepe, Ankara 06800, Turkey — In this study, the effect of the higher pressures (0-100GPa) on the electronic structure was investigated for an ordered structure of Li_xBC phase. And also, the stoichiometric effect was examined by the first principles calculations in terms of the metallic behaviour for the range of $0 \leq x \leq 1$. It was observed that the density of states near the Fermi level decreases depending on the pressure and the energy gap above the Fermi level contracts for the higher pressure values for especially $Li_{0.5}BC$ compound predicted as a superconductor [1-3]. DOS is extremely sensitive to the Li stoichiometry and the unit cell volume. The pressure has the different effect on the electronic structure of $Li_{1.0}BC$ system behaviour for the same pressure range by contrast with the nonstoichiometric LiBC.
[1] Rosner H.et al., PRL 88, 12, 2002.
[2] Singh P.P. et al., Solid State Comm., 124,25-28, 2002.
[3] Dewhurst J.K. et al., PRB 68, 020504(R), 2003.

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