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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$_x$BC phase. And also, the stoichiometric
effect was examined by the first principles calculations in terms of the metallic
behaviour for the range of 0 ≤ x ≤ 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.


Engin Ozdas
Advanced Materials Research Group, Physics Department,
Hacettepe University, Beytepe, Ankara 06800, Turkey

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