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EFFECTS OF COLLAPSE MAGNETIC UNDER PRESSURE IN IRON BORIDES



Ahmed Gueddouh
Effects of collapse magnetic
under pressure in iron borides

Condition: New. Publisher/Verlag: Noor Publishing | First-principles calculations are performed to study pressure effects on structure, magnetic and mechanical properties of FexB ($x=1, 2, 3$) compounds using density functional theory (DFT) within GGA approximation. The three structures are studied in the pressure range from 0 to 90 GPa, in order to predict the critical transition pressure from magnetic to nonmagnetic states (NM) and a possibility of superconductivity in this state was predicted. Mechanical anisotropies in both cases are discussed by...

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- Authored by Gueddouh, Ahmed
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