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Band structure calculations of Mo_2BC under pressure R. FALCONI, UJAT, F. ALVAREZ, IMP, R. ESCAMILLA, R. ESCUDERO, UNAM — Mo_2B is a superconductor with a Tc of about 5.8 K and a body centered tetragonal cristalline structure. When carbon is added to the structure it is formed the intermetallic Mo_2BC compound, which is a superconductor with a Tc of about 7 K and has a crystalline face centered orthorhombic structure. In this work we make ab initio calculations of the electronics bands for Mo_2BC at several pressures up to 5 GPa in order to explain why chemical pressure, generated by decreasing the carbon concentration, decreases T_C in a non linear rate. The density of state at the Fermi level is reduced in a non monotonic way suggesting some correlation. We complement the study with high pressure electrical resistivity measurements up to 4.8 GPa which reveal a decreasing of Tc at the rate dT_C/dP = - 0.03 K/GPa.

R. Falconi
UJAT

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