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MgB_2: doped or with pressure, four systems same behaviour

PABLO DE LA MORA, SABINA RUIZ-CHAVARRIA, ULISES ESTEVEZ, Fac. de Ciencias, GUSTAVO TAVIZON, Fac. de Quimica, UNAM, Mexico, D.F. — MgB_2, the intermediate T_c superconductor, can be doped with carbon, aluminium and scandium and it has been also studied experimentally under pressure, in these four cases T_c diminishes. In previous studies we have shown, with electronic structure calculations, that when Mg is substituted with Sc $[(Mg,Sc)B_2]$ the drop of T_c can be associated with the loss of electrical anisotropy of the σ-bands [1]. When Mg is substituted with Al $[(Mg,Al)B_2]$ or B is substituted with C $[Mg(B,C)_2]$ then, with a change of doping scale, a common T_c curve is obtained for both systems, comparison with the σ-DOS shows that T_c drop is due to σ-band-filling and to σ-band anisotropy loss [2]. In further studies we have found that both these features, σ-band anisotropy reduction and the loss of σ-band-carriers, can be associated to the drop of T_c in these three doped systems $[Mg(B,C)_2$, $Mg,Al)B_2$ and $(Mg,Sc)B_2]$ and in MgB_2 under pressure. All these studies show that: (a) with a change of doping scale then T_c in both the C and Al doped systems follows the same curve which is very close to the σ-DOS; (b) for the four systems both the σ-band anisotropy and the number of σ-carriers are two fundamental physical properties of the relatively high T_c in MgB_2. [1] J. Phys.: Condens. Matter 18 (2006) 1403-1412 [2] cond-mat/0606019

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