Abstract Submitted for the MAR09 Meeting of The American Physical Society

 MgB_2 under pressure; band-filling, phonon hardening and electrical anisotropy JESUS VAZQUEZ, SABINA RUIZ-CHAVARRIA, PABLO DE LA MORA, Fac. de Ciencias, Universidad Nacional Autonoma de Mexico — The electrical two-dimensional character has been accepted as an important factor in the high T_c superconductors. In MgB_2 it is the almost two dimensional σ -bands that are responsible for the superconductivity. On the other hand in MgB_2 the band-filling and phonon hardening have been found to be the responsible for the high T_c [1]. But previous calculations [2] have shown that with pressure both, electrical anisotropy and T_c are reduced. Thus the question arises: Is the electrical anisotropy, together with band-filling and phonon hardening, also responsible of the high T_c in MgB_2 ? Using the WIEN2k package the MgB_2 superconductor is analyzed as function of pressure. At each pressure the cell parameters are optimized and the σ -DOS, the E_{2q} -phonons and the electrical anisotropy of the σ -bands are calculated and, with the use of the Hopfield expression, are analyzed to see what the correlation of these elements with T_c is. [1] J Kortus, Physica C 456 (2007) 54-62 [2] U Esteves and P de la Mora, Rev. Mex. Fis. 53 (2007) 95-98

> Carlos Cosio-Castaneda Fac. de Quimica, Universidad Nacional Autonoma de Mexico

Date submitted: 10 Dec 2008

Electronic form version 1.4