Studying the electronic structure in pure and electron doped MgB$_2$\textsuperscript{1} Y. ZHU, R.F. KLIE, L. WU, J.C. ZHENG, Center for Functional Nanomaterials, L.D. COOLEY, Dept. Cond. Matt. Phys. & Mat.Sci., Brookhaven National Lab — We use high-energy electrons to reveal electronic structure information to understand the effects of electron doping in MgB$_2$ superconductors. Angle-resolved electron energy-loss spectroscopy was used to investigate the difference in the excited states, while image-coupled quantitative electron diffraction was used to map the valence electron distribution, in pure and Al-doped MgB$_2$. The results were compared with density functional theory calculations. We found significant changes in the B K-edge fine structure as a function of electron doping concentration, suggesting the corresponding $\sigma$ and $\pi$ bands are being filled simultaneously. The filling of the $\sigma$-band states near the Fermi level reduces the critical temperature $T_c$ of highly doped MgB$_2$ to a level comparable to that of other $\pi$-band superconductors such as intercalated graphite. Valence electron maps reveal that electron doping causes considerable charge transfer and accumulation in charge density between both Al-B and B-B bonds. This results in a shortened c-axis of the unit cell and higher phonon frequency, which eventually quenches superconductivity altogether. The relationship between charge transfer and inter-band scattering are also examined.

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