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First Principles studies of 122 Ferropnictide Surface[1] ALEXANDER KEMPER, P.J. HIRSCHFELD, H-P. CHENG, University of Florida — We present DFT-GGA calculations for the Ba and Sr-122 ferropnictide materials on the effect of surfaces on the electronic structure. It has been established that there is a strong modulation of the electronic structure by the Fe-As distance, which decreases near a free surface due to surface reconstruction. Indeed, we see significant changes of both Fermi velocities and Fermi surfaces due to these effects for both the paramagnetic and collinear spin density wave states. These changes of the electronic structure, which we exhibit here, will be crucial for the interpretation of surface probes like ARPES and STM.

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