List of Figure Captions

Figure 1. Comparison of the density of states as a function of energy obtained ab initio to the density of states for a parabolic approximation to the valence and conduction bands.

Figure 2. Calculated values of E_F as a function of temperature for three different density of states approximations in the intrinsic (upper three curves) and heavily doped (bottom three curves) regimes. The dashed lines corresponds to E_F using the ab initio density of states, the solid lines are determined with Green's N_C and N_V and the dotted lines were obtained with the $T^{3/2}$ using the data from Sze.

Figure 3. Comparison of calculated dopant enhanced solubility of Fe in Si as a function of temperature using different density of states approximations while assuming E_T remains at a constant fraction of EG. The doping level is $N_A=1.5x10^{19}$ which corresponds to the doping level of the Si investigated by McHugo et al (solid squares denote their data points). With the exception of the fine dotted line, all calculations were performed using Fermi-Dirac statistics to calculate E_F. A comparison between the fine dotted line (E_F obtained with the Boltzmann approximation for the $T^{3/2}$ model) and the dashed double dot line illustrates the error generated using the Boltzmann approximation. The solid line represents the intrinsic Fe solubility.

Figure 4. Comparison of calculated dopant enhanced solubility of Fe in Si for different temperature dependencies of E_G. E_T was held a constant fraction of the gap and we use the $T^{3/2}$ model for effective density of states. The dashed line was calculated using the Varshni relation for E_G with the parameters of Alex et al while the dotted curve calculation relies on the extrapolation of a semi-empirical model for E_G.

Figure 5. Comparison of calculated dopant enhanced solubility of Fe in Si for different temperature dependencies of the Fe defect level, E_T, in the gap. Dotted line was calculated assuming that E_T is a constant distance from the valence band edge. For the dot-dashed curve, E_T was held a constant fraction of the gap. The dashed curve was obtained by assuming that E_T is a constant distance from the conduction band edge. The solid line denotes intrinsic solubility.