

Abstract Submitted
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The shallow donor wavefunction in Si: Corrections to the KL effective mass theory (EMT) THEODORE CASTNER — The ENDOR data of Hale & Mieher¹ (HM) provides detailed information on $\psi^*\psi(\mathbf{R}_{nrm})$ at nearly 25 lattice sites for P, As, & Sb. Ivey & Mieher²(IM) have given the most comprehensive calculation of $\psi(\mathbf{r}) = \sum \mathbf{A}(\mathbf{k})\mathbf{u}_k(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$ featuring a complex $\mathbf{A}(\mathbf{k})$ (and $\mathbf{u}_k(\mathbf{r})$) and higher conduction bands. IM could identify most of the sites and reduce the rms error between theory values and experimental results from 60% to 11%. However, the IM results are poor for the (1,1,1) site [shell E] and don't provide clear evidence for subsidiary minima³ (L_1, Γ_2') from their region IV in the BZ. A reliable calculation of matrix elements $\langle L_1[U(\mathbf{r})]\Delta_{1,min} \rangle$ is difficult because of the complicated core potential in the central cell. Using the equidistant matched lattice pair data [(3,3,3) & (1,1,5); shells C and Q] provides a good estimate of the % admixture from the L_1 minima, somewhat smaller than in [3]. The IM $\text{Im}\mathbf{A}(\mathbf{k})$ and the L_1 minima both provide corrections to the uniaxial strain i_d parameter⁴. A data analysis for the odd lattice sites improves the agreement between theory and experiment. Important remaining theoretical issues will be discussed and new ENDOR experiments will be proposed. The corrections to EMT are important, but are smaller than implied in IM. 1) E.B. Hale & R.M. Mieher, Phys.Rev.184, 739, 751 (1969). 2) J.L. Ivey & R.M. Mieher, Phys.Rev.B11, 822 (1975). 3) T.G. Castner, Phys.Rev.B2, 4911 (1970). 4) E.B. Hale & T.G. Castner, Phys.Rev.B1, 4763 (1970).

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