Theoretical study of the Cu\textsubscript{PL} defect in Si ALEXANDRA CARVALHO, University of Aveiro, STEFAN K. ESTREICHER, Texas Tech University

— Copper is a common contaminant in Si processing. When in supersaturation, a fraction of 1% of the Cu in the sample forms an electrically-active defect easily seen by photoluminescence. This Cu\textsubscript{PL} defect in Si has a no-phonon line at 1014 meV. It has long been believed to consist of an interstitial copper (Cu\textsubscript{i}) weakly bound to a substitutional copper (Cu\textsubscript{s}) : The \{Cu\textsubscript{s}Cu\textsubscript{i}\} pair. However, PL studies in isotopically pure $^{28}$Si crystals have shown that the defect contains not two but four copper atoms [1]. We examine the possibility that the core of the defect consists of not one but two adjacent substitutional Cu atoms. This core traps two Cu\textsubscript{i} atoms, resulting in defect with $D_{3d}$ symmetry. We will discuss its formation mechanism and stability, and show that they are consistent with the conditions at which Cu\textsubscript{PL} is observed. If this model is correct, then then DLTS lines associated with Cu\textsubscript{s} should be re-assigned to \{Cu\textsubscript{s}Cu\textsubscript{s}\}.