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Deep Level Tight-Binding Model for Transition Metal Dopant States in Diamond VICTORIA KORTAN, CUNEYT SAHIN, MICHAEL FLATTÉ, University of Iowa Department of Physics and Astronomy — Diamond is a promising system for quantum information processing [1], providing the possibility of single-spin-photon entanglement, as well as the potential for high-speed spin manipulation at room temperature (such as has been demonstrated for the electronic spin associated with an NV center [2]). Ion implantation has been demonstrated for controllable positioning of NV centers; in principle other dopants could be so implanted as well. For example, transition-metal dopants could potentially be used as optically and electrically active single spin qubits [3]. Here we use a deep level tight binding model to study the electronic trends and defect wave functions of transition-metal dopants in diamond. Starting with the Green's functions of homogeneous diamond (within an spds* tight-binding model), a Koster-Slater approach is used to evaluate the defect state. This work is supported by an AFOSR MURI.

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