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Transition-Metal Dopants in Tetrahedrally Bonded Semiconductors

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Single and few defects can control the properties of nanomagnetic systems and thus are of great importance to nanometer scale systems [1]. Diamond provides an advantageous system to study these defects due to its extended spin coherence times [2], the presence of optically addressable spin centers and the progress that has been made with ion implantation [3]. The negatively charged nitrogen vacancy center is an especially attractive optically addressable spin center in diamond and there have been many impressive experimental demonstrations of optical spin initialization, manipulation, coupling and read-out [4]. Also of interest are transition-metal dopants with partially-filled d-levels which offer the possibility of electrical manipulation due to their large spin-orbit interaction [5,6]. These partially-filled d-levels split in symmetry of the diamond lattice into e and t_2 symmetry states. These two states are predicted to have different spatial extents [4,5] and this in turn affects the exchange interaction between pairs of spin centers. Using an spds* tight-binding model [7] and a Greens function-based Koster Slater technique (as in [8]) we calculate the exchange interaction between pairs of transition metal spin centers and compare these with the exchange interaction between pairs of negatively charged nitrogen vacancy centers [9]. The exchange interaction is comparable between the two and suggests the relevance of transition metal spin centers in diamond. I acknowledge collaborations with C. Sahin and M. E. Flatte. This work was supported in part by an AFOSR MURI. [1] P. Koenraad & M.E. Flatté, Nat. Mat. 10, 91 (2011). [2] G. Balasubramanian, et. al. Nature Materials 8, 383 (2009). [3] D. M. Toyli, et. al. Nano Letters 10, 3168 (2010). [4] F. Jelezko & J. Wrachtrup. Phys Status Solidi A 203, 3207 (2006). [5] T. Chanier, et. al. Europhys. Lett. 99, 67006 (2012). [6] T. Chanier, et. al. Phys. Rev. B 86, 085203 (2012). [7] J.-M. Jancu, et. al. Phys. Rev. B 57, 6493 (1998). [8] J.-M. Tang & M. E. Flatte. Phys. Rev. Lett. 92, 047201 (2004). [9] V. R. Kortan et al., Phys. Rev. B 93, 220402(R) (2016).