Abstract Submitted
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spds* Tight-Binding Model for Exchange Interaction Between Transition Metal Dopants in Diamond and SiC[1] VICTORIA R. KORTAN, CÜNEYT ŞAHIN, MICHAEL E. FLATTÉ, Optical Science and Technology Center & Department of Physics and Astronomy, University of Iowa — Diamond and SiC are wide-band-gap semiconductors with long-lived spin lifetimes[1,2] and promising for quantum information technology device design. Spin initialization, manipulation and readout has already been demonstrated for the NV center in diamond[3] and the divacancy in SiC[4]. Transition metal spin centers offer additional benefits in tetrahedral hosts due to the crystal field splitting of the d-states into localized and extended states. For example, the application of strain in diamond allows switching between two spin states of a single Ni dopant[5]. Here we use a spds* tight-binding model including spin-orbit interaction to describe transition metal spin centers in diamond and 3C-SiC as well as the NV center in diamond and divacancy in 3C-SiC. The energy levels for an isolated dopant are taken from experiment, when available, and density functional theory calculations otherwise. We calculate and compare the wavefunctions of these spin centers, as well as the strength of the exchange interaction between pairs of them.

[1] A. Falk, et al, Nature Comm. 4, 1819 (2013).
[2] G. Balasubramanian, et al, Nature Mat. 8, 383 (2009).
[3] N.B. Manson, et al, Phys. Rev. B 74, 104303 (2006).
[4] W.F. Koehl, et al, Nature 479, 84 (2011).
[5] T. Chanier, et al, EPL 99, 67006 (2012).

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