Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

spds* Tight-Binding Model for Transition Metal Dopants in SiC[1]

VICTORIA R. KORTAN, CÜNEYT ŞAHIN, MICHAEL E. FLATTÉ, Optical Science and Technology Center & Department of Physics and Astronomy, University of Iowa, Iowa City, IA, USA — SiC is a well known, wide-band-gap semiconductor with excellent chemical, thermal and mechanical stability. These traits make it an attractive material for high temperature, hostile environment, high power and high frequency device design[1]. A necessary step in the development of SiC technology is the understanding and subsequent control of point defects[2]. In addition to altering optoelectronic properties, single dopants can add effects dependent on the specific dopant species. In particular the d-states of transition metal dopants have been predicted to allow the control of the single Ni spin state with the application of strain in diamond [3] and single Fe dopants in GaAs have a core transition that can be manipulated by a STM and produce a decrease in tunneling current[4]. Here we choose a first and second nearest neighbor spds* tight-binding model to calculate the electronic trends and defect wavefunctions of transition metal dopants in 3C-SiC. Additionally we calculate the exchange interaction between pairs of dopants.

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[1]This work was supported by an AFOSR MURI.

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Date submitted: 15 Nov 2013 Electronic form version 1.4