Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Excited States of the divacancy in SiC MICHEL BOCKSTEDTE, THOMAS GARRATT, University of Erlangen-Nueremberg, Germany, VIKTOR IVADY, Linkoeping University, Sweden and Wigner Research Centre of Physics of the Hungarian Academy of Sciences, Hungary, ADAM GALI, Wigner Research Centre of Physics of the Hungarian Academy of Sciences, Hungary and Budapest University of Technology and Economics, Hungary — The divacancy in SiC - a technologically mature material that fulfills the necessary requirements[1] for hosting defect based quantum computing - is a good candidate for implementing a solid state quantum bit. Its ground state is isovalent to the NV center in diamond as demonstrated by density functional theory (DFT).[2] Furthermore, coherent manipulation of divacancy spins in SiC has been demonstrated.[3] The similarities to NV might indicate that the same inter system crossing (ICS) from the high to the low spin state is responsible for its spin-dependent fluorescent signal. By DFT and a DFT-based multi-reference hamiltonian we analyze the excited state spectrum of the defects. In contrast to the current picture of the spin dynamics of the NV center, we predict that a static Jahn-Teller effect in the first excited triplet states governs an ICS both with the excited and ground state of the divacancy.

[1]J. R. Weber *et al.*, PNAS **107**, 8513 (2010).
[2]A. Gali, phys. status solidi (b) **248**, 1337 (2011); J. P. Gross *et al.* **77**, 3041 (1996).
[3]F. Koehl *et al.*, Nature**479**, 84 (2011).

Michel Bockstedte
Theoretische Festkoerperphysik, University of Erlangen-Nueremberg,
Staudtstr. 7B2, 91058 Erlangen, Germany

Date submitted: 14 Nov 2013 Electronic form version 1.4