Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

***Ab initio* electron paramagnetic resonance study of 3C-SiC/SiO_2 interfaces in SiC-nanofiber based solar cells**[1] TAUFIK ADI NUGRAHA, Max-Planck-Institut fuer Eisenforschung, UWE GERSTMANN, WOLFGANG GERO SCHMIDT, University of Paderborn, STEFAN WIPPERMANN, Max-Planck-Institut fuer Eisenforschung — Semiconducting nanocomposites, e. g. hybrid materials based on inorganic semiconducting 3C-SiC nanofibers and organic surfactants, provide genuinely novel pathways to exceed the Shockley-Queisser limit for solar energy conversion. The synthesis of such functionalized fibers can be performed completely using only inexpensive wet chemical solution processing. During synthesis a thin passivation layer is introduced between the SiC-fiber and surfactants, e. g. the native oxide, whose atomistic details are poorly understood. In this study, we utilize unpaired spins in interfacial defects to probe the local chemical environment with *ab initio* EPR (Electron Paramagnetic Resonance) calculations, which can be directly compared to experiment. Considering a wide variety of possible interfacial structures, a grand canonical approach is used to generate a phase diagram of the 3C-SiC/SiO_2 interface as a function of the chemical potentials of Si, O and H, to provide favorable interfacial structures for g-tensor calculations. This study provides directions about specific types of interfacial defects and their impact on the electronic properties of the interface. The authors wish to thank S. Greulich-Weber for helpful discussions.

[1]S. W. acknowledges BMBF NanoMatFutur Grant No. 13N12972.

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Date submitted: 06 Nov 2015 Electronic form version 1.4