Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

EPR parameters of the dangling bond defect in crystalline and amorphous silicon: A DFT-study GERNOT PFANNER, CHRISTOPH FREYSOLDT, JÖRG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Germany — Thin-film a-Si:H solar cells are considered as low-cost alternatives to bulk crystalline silicon (c-Si) solar cells. A disadvantage of these devices is that their efficiency is severely limited by light-induced defects (Staebler-Wronski effect). In this context, electron-paramagnetic resonance (EPR) is a key technique to probe for the local atomic structure of defects with unpaired spins such as the silicon dangling bond. However, the assignment of the EPR signal to a specific defect structure requires comparison to theoretical models. Using density-functional theory, we address structure-property relationships by combining systematic studies for idealized dangling-bond models in c-Si with a statistical analysis of a variety of dangling bonds in a-Si:H supercells. Our studies reveal the influence of the local geometry on sp-hybridization and delocalization. Yet, the structural variability of a-Si:H cannot be captured by these idealized defect models alone. Rather, our calculations indicate that a relatively broad distribution of dangling-bond like structures gives rise to the experimental signal supporting a recent re-evaluation of EPR parameters from multifrequency EPR.

Christoph Freysoldt
Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Germany

Date submitted: 18 Nov 2010 Electronic form version 1.4