

Abstract Submitted
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The influence of pressure on defects in amorphous silicon¹ JEF-FREY GROSSMAN, LUCAS WAGNER, University of California, Berkeley — Amorphous silicon(a-Si) thin-film solar cells are promising materials for solar cells, but they suffer from the Staebler-Wronski effect (SWE), in which the efficiency degrades over the course of a few hours of light exposure. While there has been progress in mitigating this effect through sample preparation, there is still no clear microscopic explanation for the degradation. We have used first principles density functional theory and highly accurate quantum Monte Carlo calculations to investigate the effect of pressure on different types of defects present in a-Si. Our calculations show that the effect of pressure on a-Si is strongly dependent on the particular type of defect, and they further may provide new ways to experimentally determine the dominant defect type. We also report on the effect of pressure on the simplest reaction in a-Si: a bond switch between two neighboring Si atoms, which could be an important element in the understanding of the SWE [1]. [1] L.K. Wagner and J.C. Grossman. PRL (in press)

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