Hydrogen diffusion and its consequences in light exposed a-Si:H

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Light-induced degradation of photovoltaic cells has been extensively studied in recent decades. However, the underlying physical and chemical processes are still not fully understood. In this work, using a first principles molecular dynamics simulation technique, we present: a) a direct ab-initio simulation of the response of a-Si:H to light exposure, b) a tendency to create dihydride structures upon light excitation, and c) a comparison of our results with a recent NMR experiment.