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Structure and Electronic Properties of a-Si:H Investigated with Quantum Simulation

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Abstract **-** In order to investigate various properties of hydrogenated amorphous silicon (a-Si:H) for improvement of low conversion efficiency of solar cells, a series of quantum simulations based on the density functional theory combined with the tight binding model were performed for a-Si:H with various hydrogen concentrations and fabrication methods. The radial distribution function (RDF) for Si-Si pairs indicates that samples with higher H concentration (20% and 25%) give a better structure, but the RDF of Si-H pairs suggests that samples with lower H concentration (14% and 20%) may give better properties. The coordination number analysis indicates that more defects (dangling bonds and floating bonds) exist in 25% and 20% H concentration samples. Overall, a-Si:H with 14% H concentration gives most preferable structure. Samples with slower cooling rate show slightly better structure.

Keywords**:** hydrogenated amorphous silicon, structural analysis, electronic property, DOS analysis, solar cell, quantum simulation