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Hydrogen microstructure and voids in amorphous silicon hydride: A first principles study RAJENDRA TIMILSINA , PARTHAPRATIM BISWAS, University of Southern Mississippi — We study distribution of hydrogen and hydride configurations in several models of a-Si:H using first-principles density functional calculations. Motivated by recent experimental result via small angle x-ray scattering, which reveals the presence of large voids (of linear dimension up to 4 nm) in a-Si:H, we develop models for a range of concentration, and study the effect of voids on hydrogen distribution. In particular, we investigate the presence of voids in two different concentration regime: high (14 at. % and above) and low (below 14 at. %) following a recent experimental observation from infrared absorption spectroscopy . The bonding environment of H atoms, and the local electronic structure near the voids are also presented.

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