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Computational generation of void-rich hydrogenated amorphous silicon ENRIQUE GUERRERO, DAVID A. STRUBBE, Univ of California - Merced — We present computational generation of void-rich hydrogenated amorphous silicon (a-Si:H) for use in studying the electronic properties for tandem solar cells. We are specifically interested in void regions in structures of varying densities which are likely to constitute defects limiting carrier mobilities and may be implicated in the light-induced degradation of the Staebler-Wronski effect. We generate structures using the Wooten-Winer-Weaire classical-potential Monte Carlo method. We create hydrogenated structures of varying densities and study the response of the bond angle deviation ($\Delta\theta$) and average bond length and compare them to non-hydrogenated a-Si structures. We utilize comparisons of the total energy and $\Delta\theta$ to identify and avoid crystalline structures as well as a class of artifactual structures of distinctively high energy. We attempt to characterize the size and position of voids using Voronoi polyhedra and persistent homology.

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