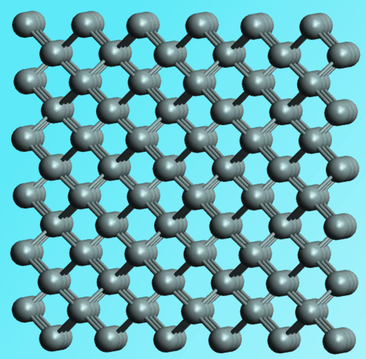
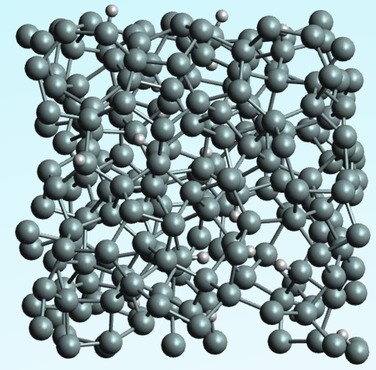


# Computational generation of void-rich hydrogenated amorphous silicon



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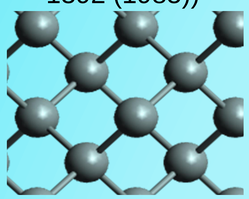
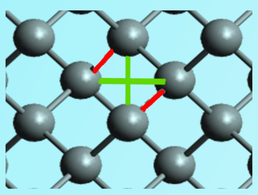
## Structure Generation

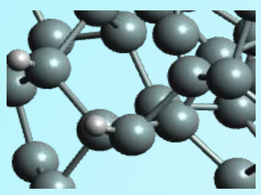
- Generation uses CHASSM (Computational Hydrogenated Amorphous Semiconductor Structure Maker), a C++ code which implements the Wooten-Winer-Weaire classical potential Monte Carlo algorithm (F. Wooten, et al., Phys. Rev. Lett. 54, 1392 (1985))



Initial 3D crystal structure



Old (red) bonds swapped for nearby ones

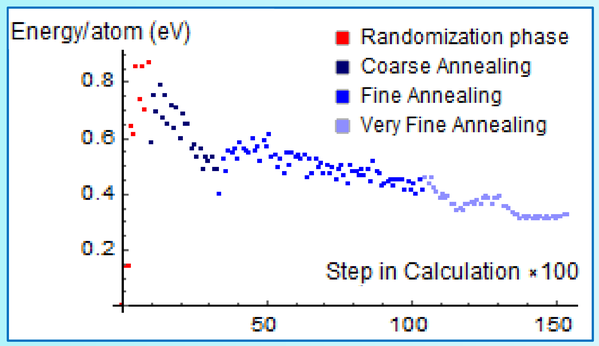


Final structure after annealing, small spheres are inserted H atoms

1. Generate crystal Si: Place atoms in a periodic, strained crystal; only bond 4 nearest neighbors
2. Hydrogenate: Randomly remove some bonds simulating hydrogen insertion and dangling bond passivation
3. Swap bonds randomly: Randomly (using Metropolis Monte Carlo probabilities) swap pairs of nearby bonds
4. Anneal: Bond switches at slowly decreasing temperature to lower energy calculated using Keating potential: (P. N. Keating, Phys. Rev. 145, 637 (1966) )

$$V = \sum_{i<j} \frac{3\,\alpha}{8\,d^2}\left(|r_{ij}|^2 - d^2\right)^2 + \sum_{\substack{i\neq j,k \\ j<k}} \frac{3\,\beta}{8\,d^2}\left(\boldsymbol{r}_{ij}\cdot\boldsymbol{r}_{ik} + \frac{1}{3}d^2\right)^2$$

bond lengths — bond angles




**Typical structure energy throughout a calculation:** After several phases, energy per atom settles on a local minimum

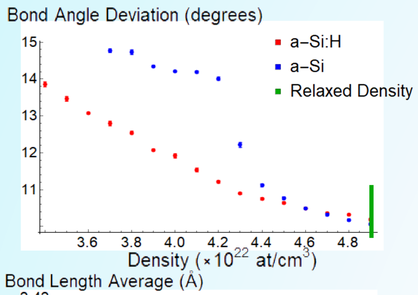
## Introduction

Void-rich hydrogenated amorphous silicon (a-Si:H) structures are likely to contain defects limiting carrier mobilities and may be implicated in the light-induced degradation of the Staebler-Wronski effect. a-Si:H is in use for cheap and flexible devices, and is promising for tandem cells with crystalline Si and organometallic perovskites. (K. A. Bush, et al., Nature Energy 2, 17009 (2017)) We study void regions and compare a-Si:H to non-hydrogenated a-Si by computationally generation at various densities. We also attempt to characterize void locations and size.

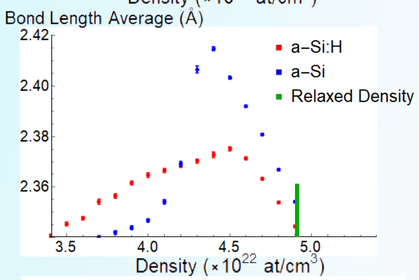

a-Si:H solar cell used in a solar powered calculator

## a-Si:H vs a-Si

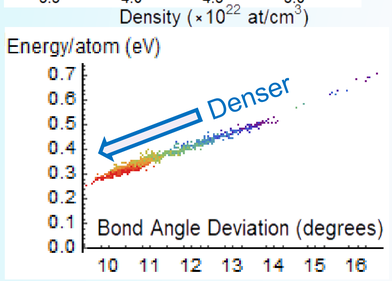
- Bond angle deviation (Δθ), energies, and average bond lengths of 60 structures (216 Si & 20 H atoms each) at different densities:




- Δθ smoothly transitions in a-Si:H when compared to a-Si



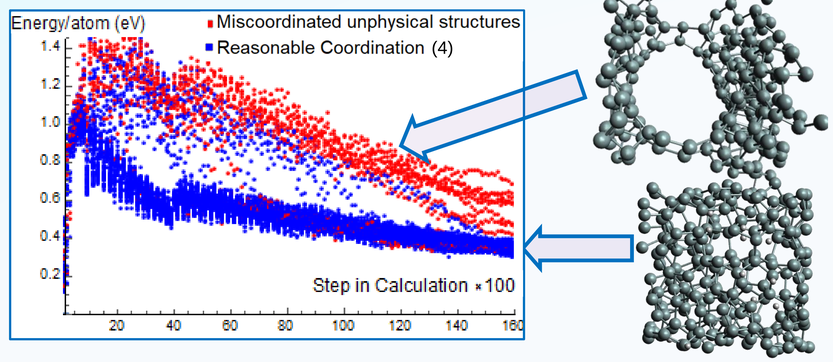

- The spike may indicate structures separate to regions of a-Si and void space




- a-Si:H structures only, red points are denser, blue-violet points are less dense

## High Energy Artifacts

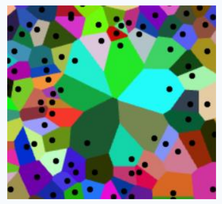
- Artifacts constitute a significant portion of data; they are highly mis-coordinated (often 10+ fold) implying they aren't realistic



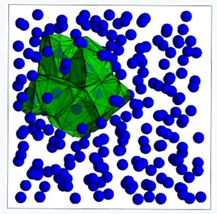

**High energy structures:** Bad structures show unphysical voids and locally dense regions. We limit randomization and exclude by energy histograms to avoid them.

## Characterizing Voids

- We use Voro++ (math.lbl.gov/voro++/) to calculate Voronoi polyhedra (VP), a geometrical tool often used to study clustering



2D VP of several sites, notice larger shapes surround the void area



Applying VP to a 3D a-Si structure; large VP are shown (green) surrounding a void. Its location is consistent with other measures.

This work is supported by UC Merced start-up funding and the Merced nAnomaterials Center for Energy and Sensing (MACES), a NASA-funded research and education center, under award NNX15AQ01, and uses computing time on the Multi-Environment Computer for Exploration and Discovery (MERCED) cluster at UC Merced, which was funded by National Science Foundation Grant No. ACI-1429783.