Electronic Supplementary Material (ESI) for Nanoscale.
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**Supplementary Information for**

# Temperature-induced nanostructural evolution of hydrogen-rich voids in amorphous silicon: A first-principles study

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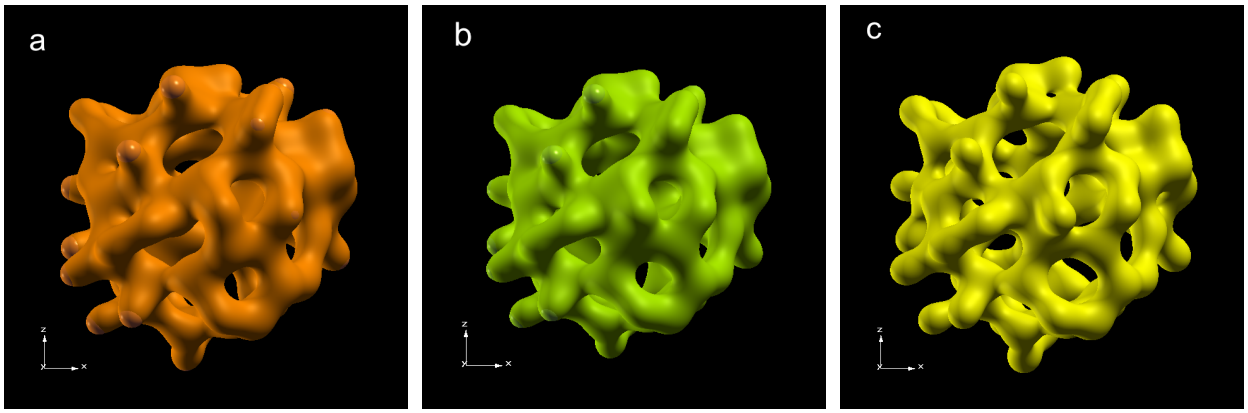


FIG. 1. A three-dimensional representation of the isosurface of a void obtained from: (a) Harris + LDA; (b) SCF + LDA; and (c) SCF + GGA. The last calculation was conducted using double-zeta (DZ) basis functions for Si atoms. The SCF + GGA yields a slightly open structure of the void, as can be seen from (c). The isosurfaces are constructed using an identical set of visualization parameters.

TABLE I. Comparison of void properties from a 1000-atom model of $a$-Si using Harris + LDA, SCF + LDA, and SCF + GGA. $R_{\mathrm{Si}}$ and $\theta$ indicate the average Si-Si nearest-neighbor distance and bond angle on the reconstructed surface of a void of radius 5 Å. $R_X$ and $\Phi_S$ are the estimated linear size from the gyrational radius ($X = g$) and the convex-hull ($X = H$) approximation, and the sphericity of the void.

| System | Basis (Si, H) | $R_{\mathrm{Si}}$ (Å) | $\theta$ (degree) | $R_g$ (Å) | $R_H$ (Å) | $V_H$ (Å$^3$) | $\Phi_S$ |
|---|---|---|---|---|---|---|---|
| Harris + LDA | SZ, DZP | $2.443 \pm 0.069$ | $108.407 \pm 17.06$ | 6.35 | 7.12 | 1245 | 0.61 |
| SCF + LDA | SZ, DZP | $2.453 \pm 0.082$ | $108.517 \pm 18.56$ | 6.31 | 7.13 | 1244 | 0.62 |
| SCF + GGA | DZ, DZP | $2.457 \pm 0.084$ | $109.307 \pm 17.58$ | 6.28 | 7.15 | 1251 | 0.59 |

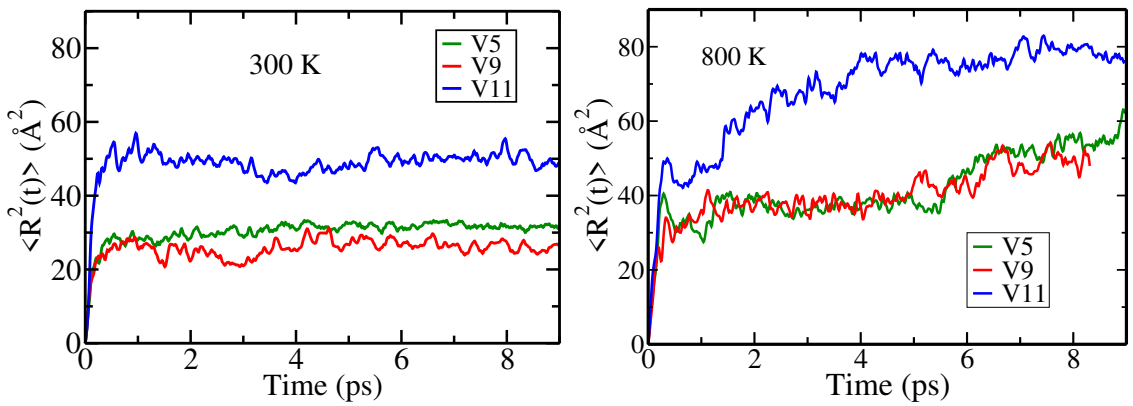


FIG. 2. The time evolution of the mean-square displacement (MSD) of hydrogen atoms inside three voids V5, V9 and V11 at 300 K (left) and 800 K (right) for a period of 8 picoseconds (ps).

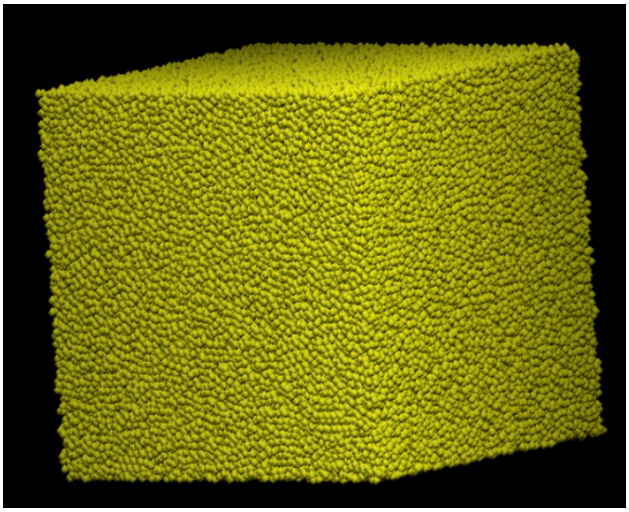

FIG. 3. The large atomistic model with 262, 400 Si atoms, which was used to generate SAXS data by introducing 12 nanometer-size voids of diameter 12 Å. The size of the model is found to be too large to render as a conventional ball-and-stick model.