

Identification of Turbostratic Twisting in Germanane

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Intensity Profiles of GeH Diffraction Pattern

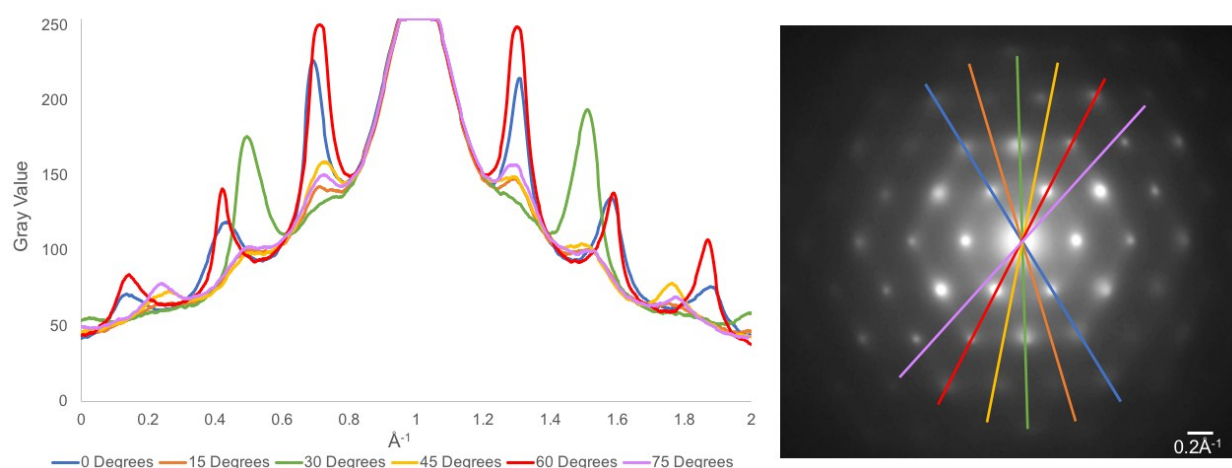


Figure S1. Intensity profiles of the GeH diffraction pattern at 15 degree increments. The orange, yellow, and pink lines indicate diffuse intensity between Bragg reflections at slightly different interplanar spacings consistent with a hexagon. If the diffuse halo were circular the interplanar spacing would be the same.

TRANSLATIONS IN GERMANANE

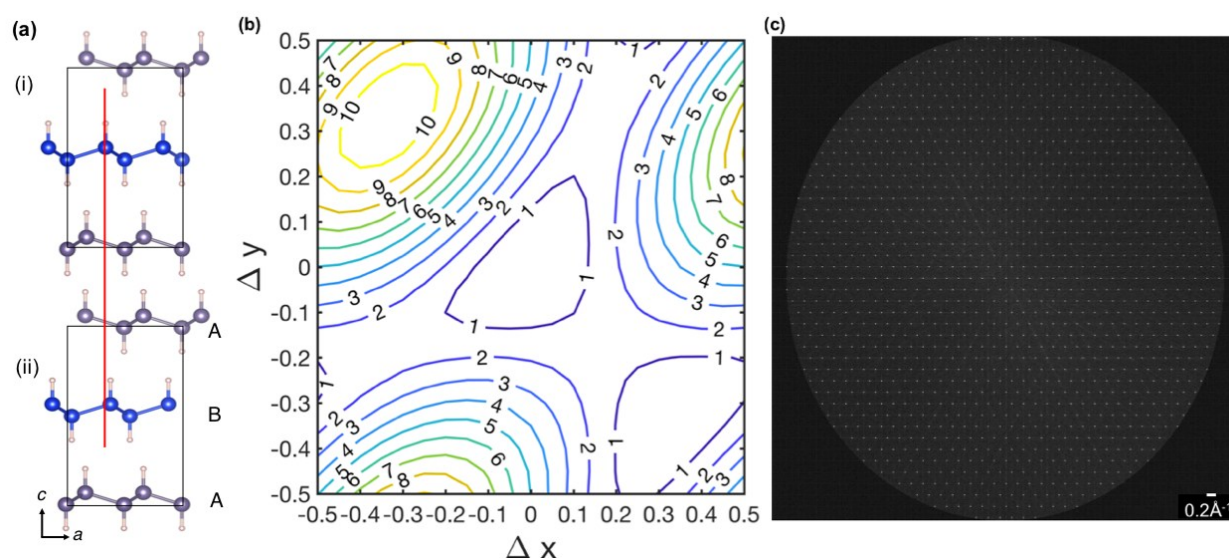


Figure S2. (a) 2H GeH structure with randomly translated layers. The red line in (a) measures the shift in [100] direction of the layer with blue Ge atoms as an example. (b) Contour plot of the translation energy (eV/Ge atom) for the structure from (a) relative to the perfect cell, calculated from DFT. (c) Simulated diffraction pattern with only translations does not contain a diffuse hexagonal halo.

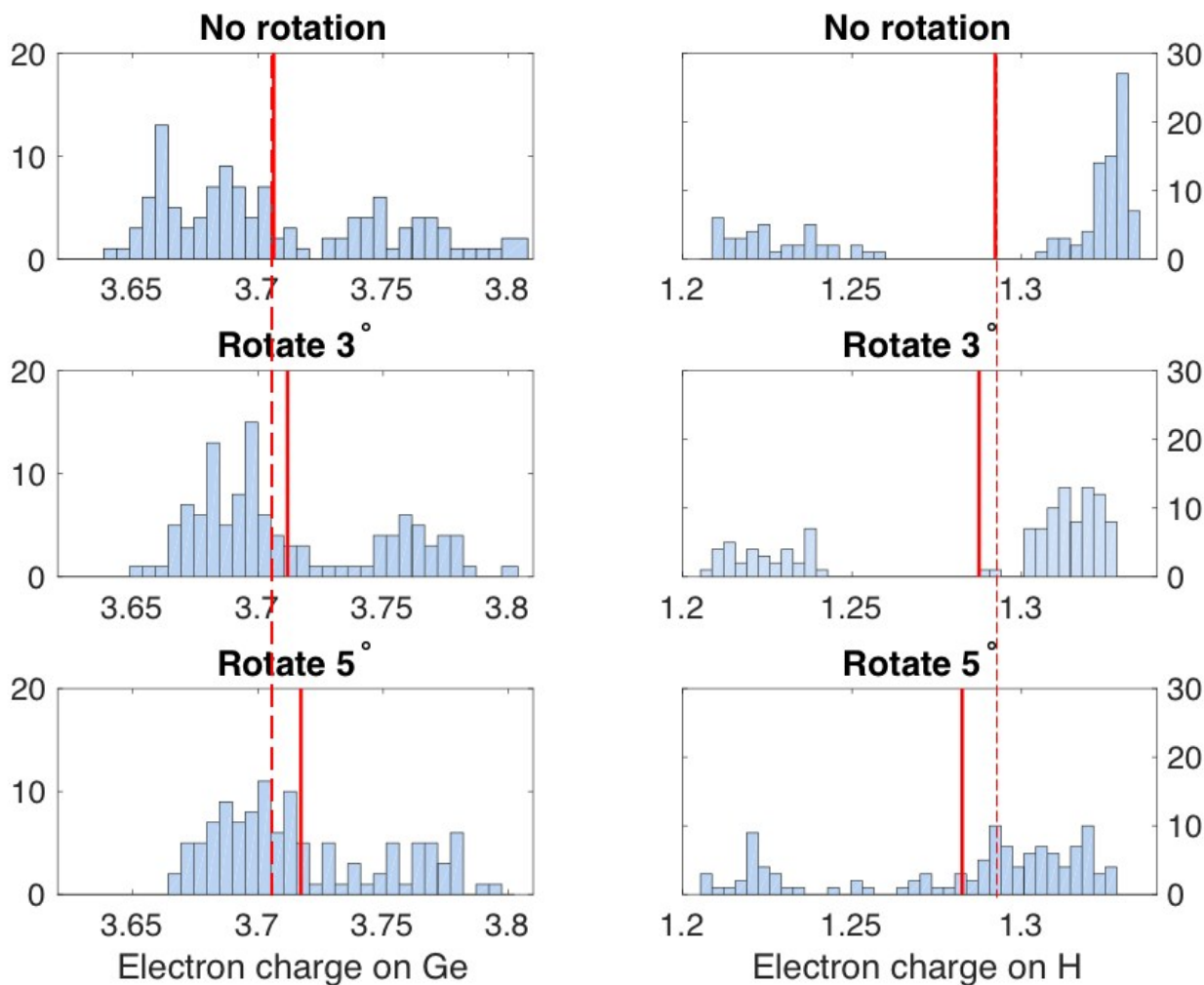


Figure S3. Histogram of DFT results for Bader charges on Ge (left panel) and H (right panel) atoms in simulation discs with 3.2 nm diameter for rotation angles of 0°, 3° and 5°. Only the atoms within a radius of 0.5 to 1.5 nm around the disc center are taken into account. The red lines represent the average electron charge. Neutral charge for Ge (H) is 4.0 (1.0).¹

DFT RESULTS FOR BADER CHARGES

DFT RESULTS FOR DENSITY OF STATES

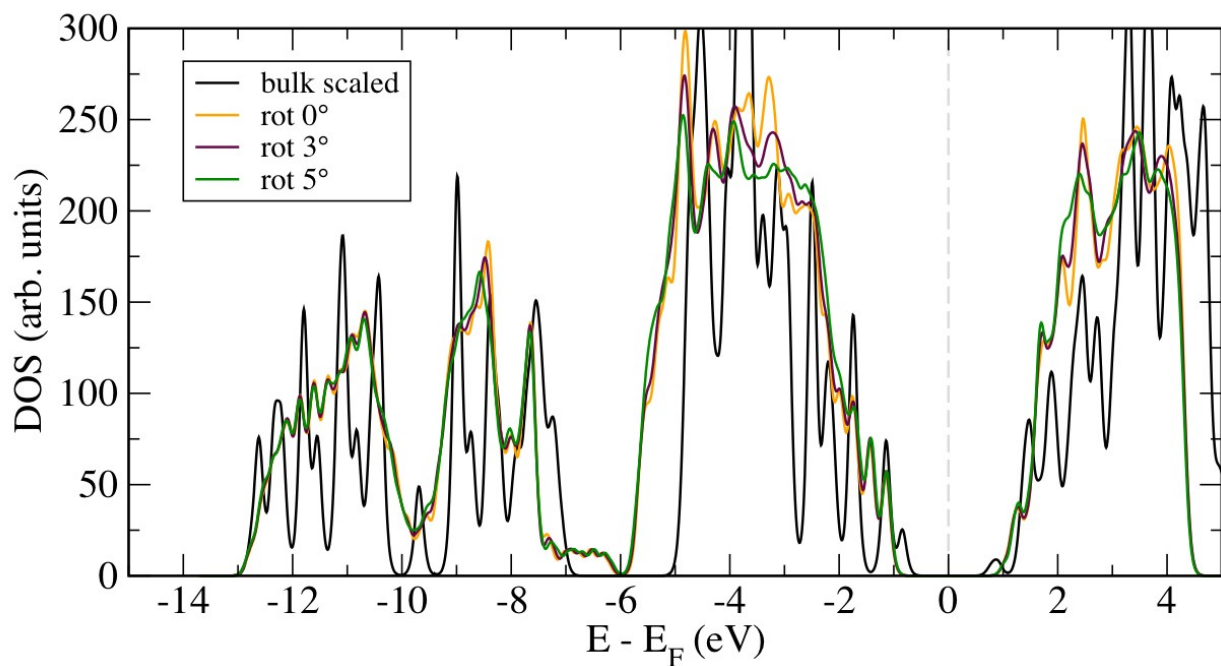


Figure S4. Comparison of density of states (DOS) between bulk 2H GeH and disk of 3.2 nm diameter with different rotation angles (black: bulk; orange: disk with no rotation; purple: disk with 3° rotation; green: disk with 5° rotation) calculated from DFT. There is an increase of ~ 0.2 eV of band gap from bulk to cluster while small rotation angle up to 5° does not significantly change the band gap.

References

- 1 G. Henkelman, A. Arnaldsson, and H. Jónsson, *Comp. Mater. Sci.* **36**, 354–360 (2006).