Stability of "Self-Interstitials" on Ge(113): STM Experiments and LDA Theory

A. Laracuente*, S. C. Erwin, L. J. Whitman

Naval Research Laboratory
Washington, DC
**email: laracuen@stm2.nrl.navy.mil*

Why Si(113) and Ge(113)?

High-index surfaces: possible substrates for electronic devices?

Of the few high-index Si and Ge surfaces with planar reconstructions, the (113) orientation is of particular interest...

At room temperature, Si(113) has a novel surface reconstruction[1]

- **Incorporates a highly-unusual six-fold-coordinated surface interstitial.**
- **The "self-interstitials" occur within every other tetramer, making the otherwise (3×1) surface (3×2).**
- **It has been proposed that at ~ 500 °C, where Si(113) turns (3×1), the surface incorporates an interstitial atom in every tetramer**

A number of groups have studied Ge(113), however, its surface reconstruction remains controversial.[2,3]

- **X-ray diffraction study concluded that Ge(113) has a similar structure to Si(113), but with the interstitials randomly distributed at the surface.**
- **An STM study concluded that the structure of Ge(113) differs from that on Si(113) (although it also proposed the presence of interstitials).**

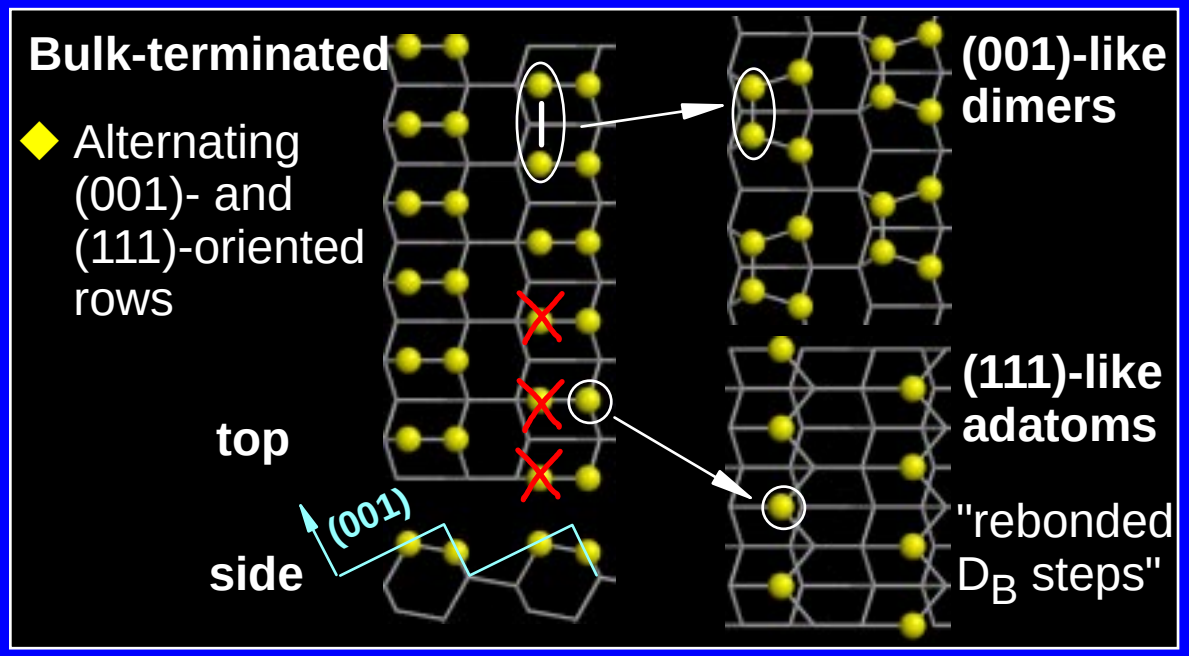
[1] J. Dabrowski, H. -J. Müssig, and G. Wolf, Phys. Rev. Lett. **73**, 1660 (1994).
[2] H. Vogler, A. Iglesias, W. Moritz, and H. Over, Phys. Rev. B **57**, 2315 (1998).
[3] Zheng Gai, R. G. Zhao, and W. S. Yang, Phys. Rev. B **56**, 12303 (1997).

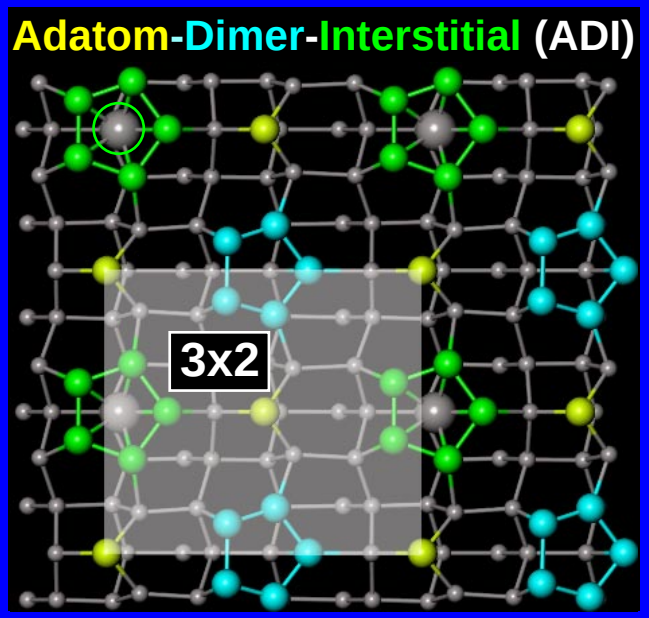
Reconstructing the (113) surface

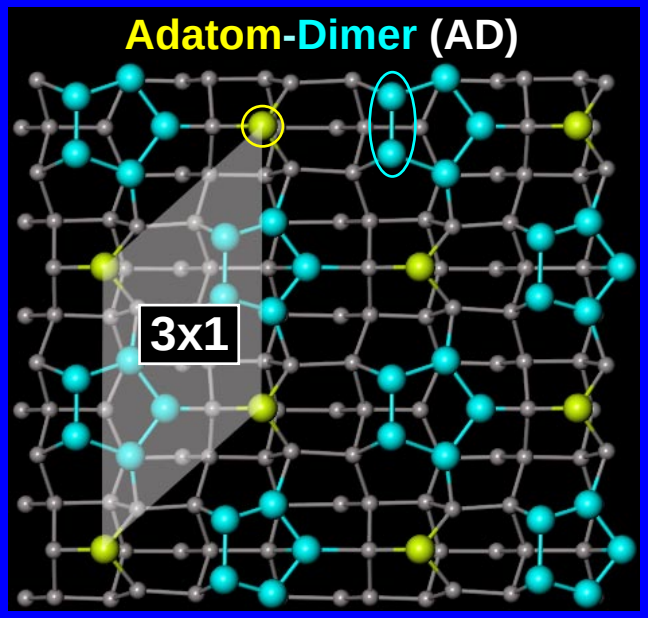
Brief history of Si(113)

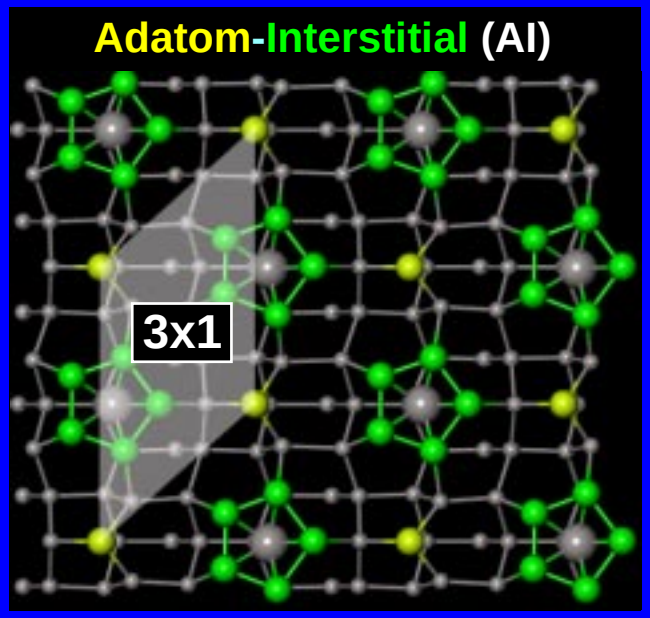
- LEED: 3x1, 3x2 (Olshanetsky '81)
- STM & models (Ranke '90; ...)
- 3x2 reconstruction (Knall '94)
- Theory & ADI model (Dabrowski '94)

Ge(113)-(3×1): AD or AI model ?







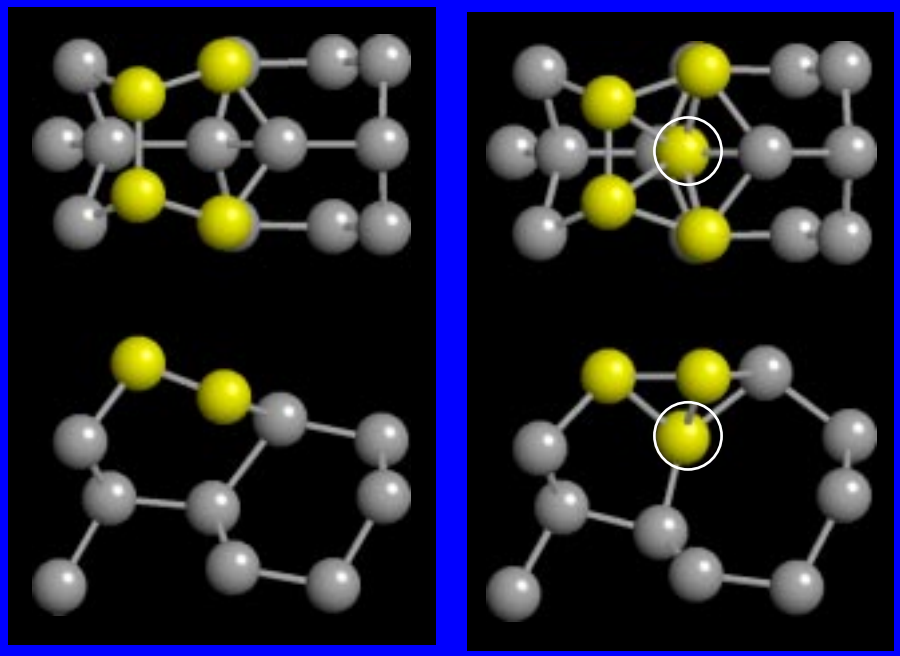


Si(113)-(3×2) and the [110]-split self-interstitial

(113) surface dimer

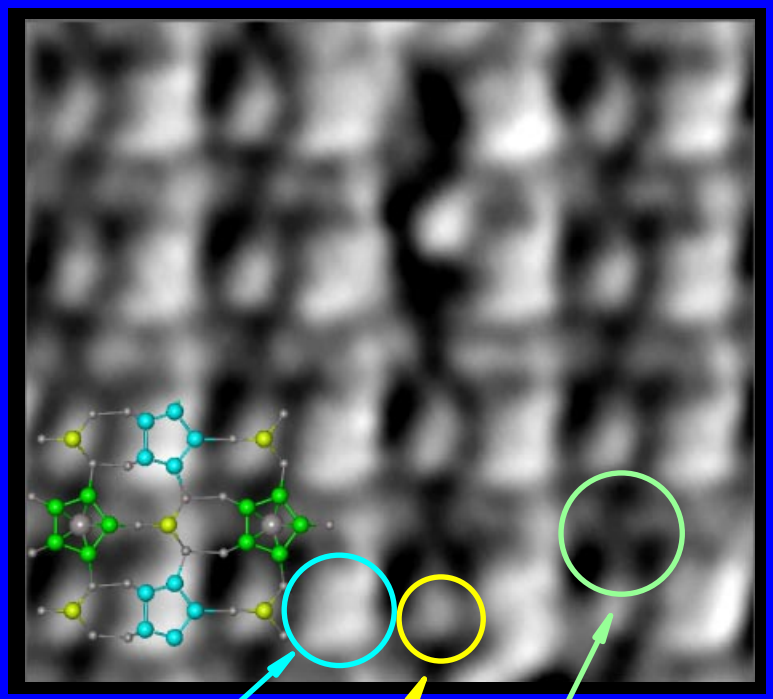
without interstitial

with subsurface interstitial



Si: E_F = 4.3 eV
Ge: E_F = 3.3 eV

Filled-state STM image



Interstitial makes tetramer dark !

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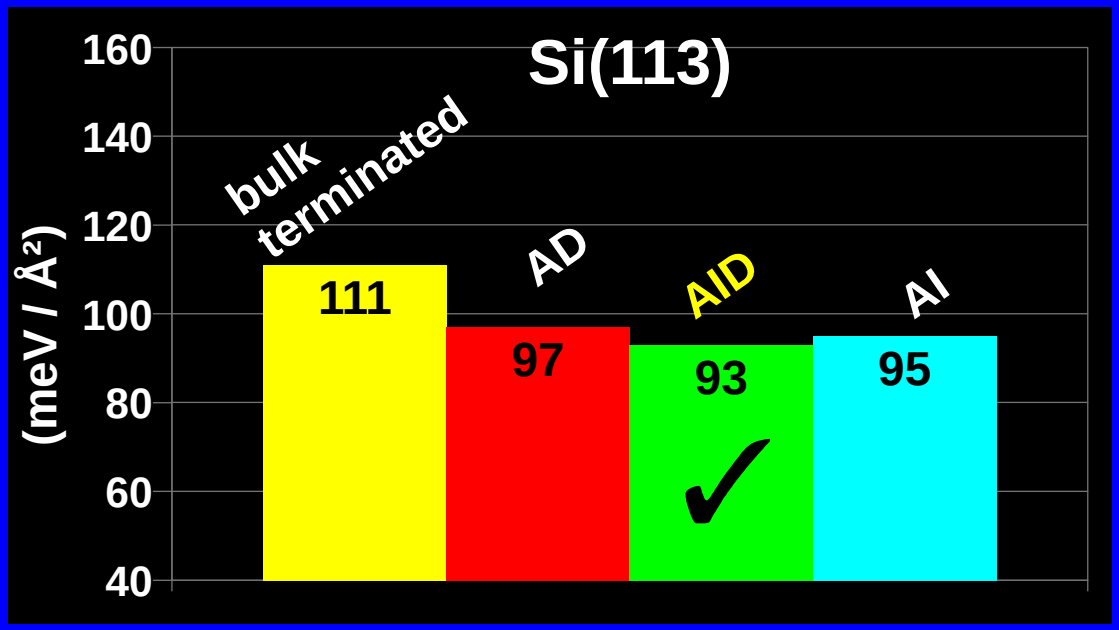
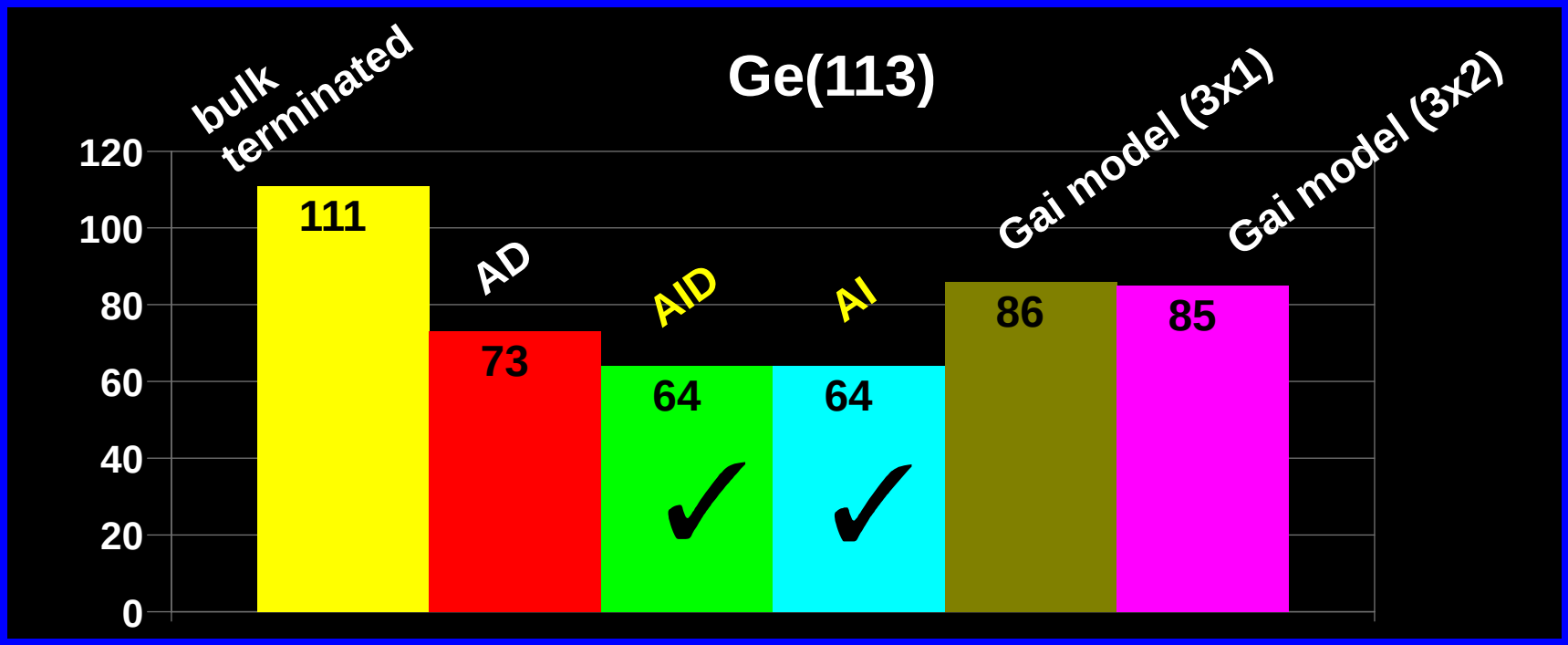
Theoretical (LDA) surface energies

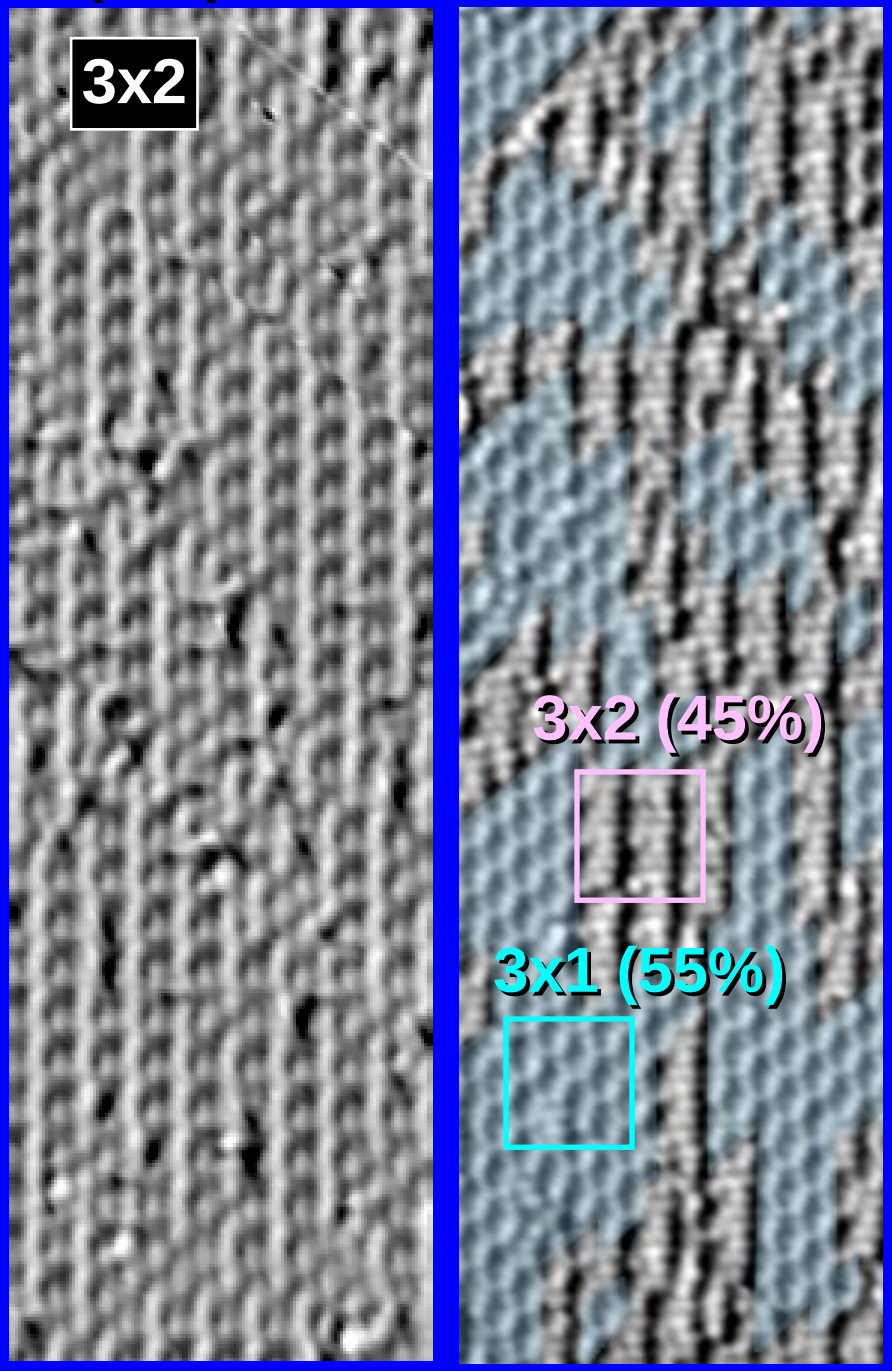


Calculations by Steve Erwin

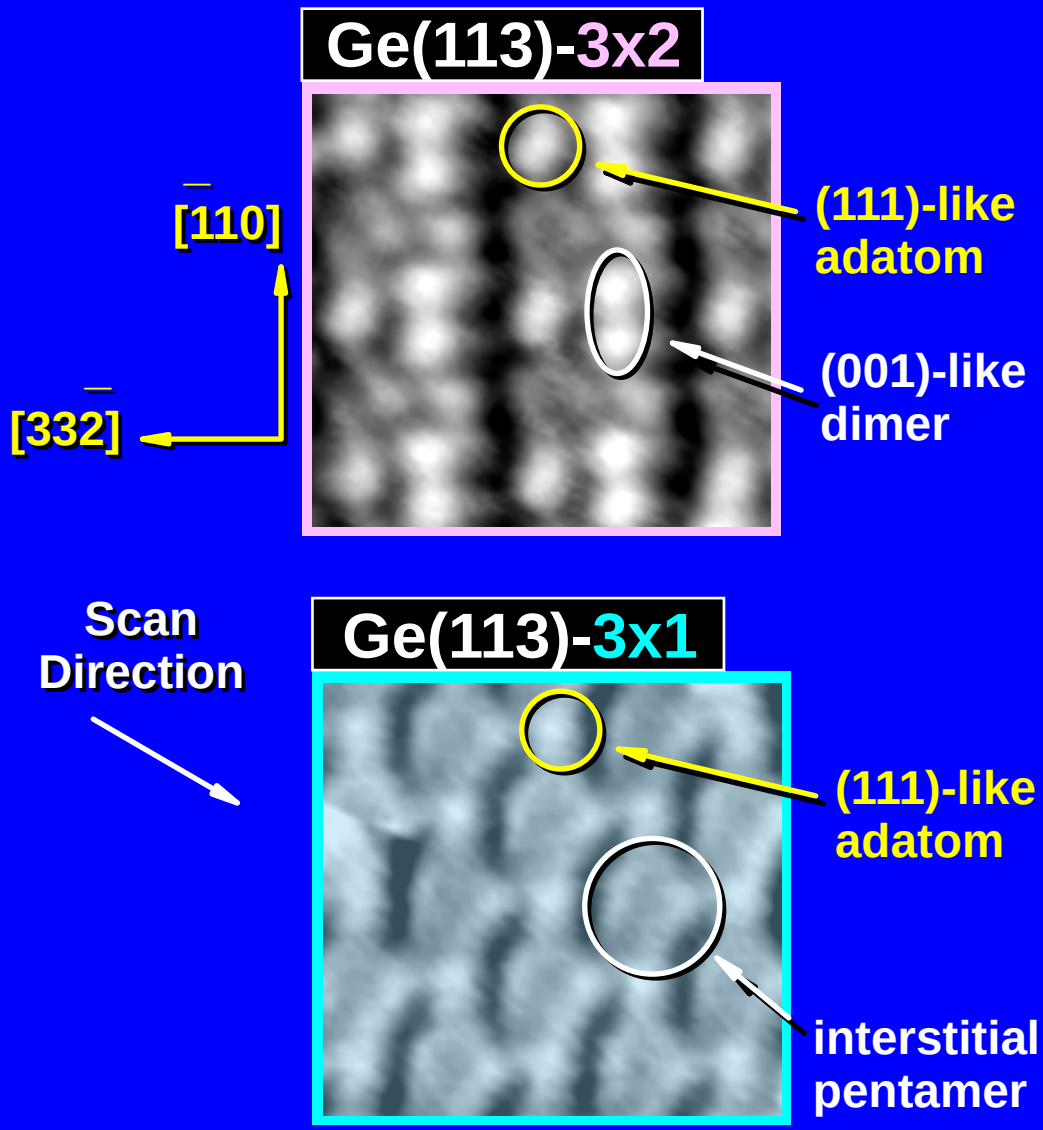
Local-Density Approximation (LDA)
Troullier-Martins pseudo potentials (+-)
8 layers super cell slab
Vacuum thickness: 4 layers
Energy cutoff: 8 Ry (Si); 15 Ry (Ge)
Brillouin-zone sampling: 4 k-points
Software: `FHI96MD` (Bockstedte, Kley, & Scheffler)



Morphology of Si(113) vs. Ge(113)



Filled States (2 V) 100 Å × 320 Å



About 55% 3×1

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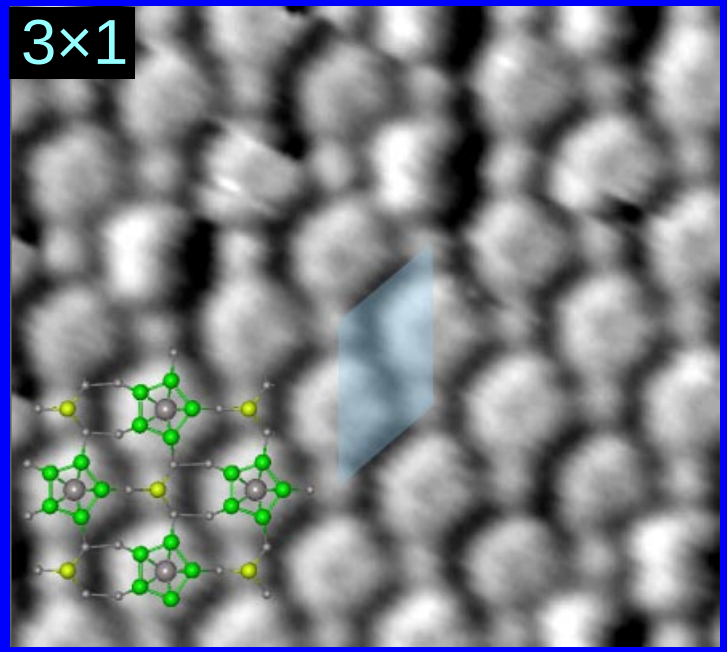
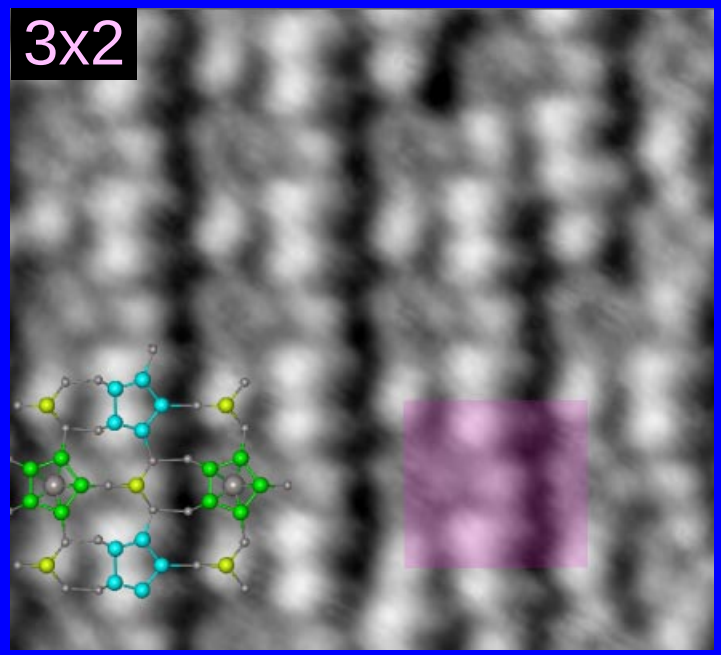
Ge(113) 3×1«--» 3×2





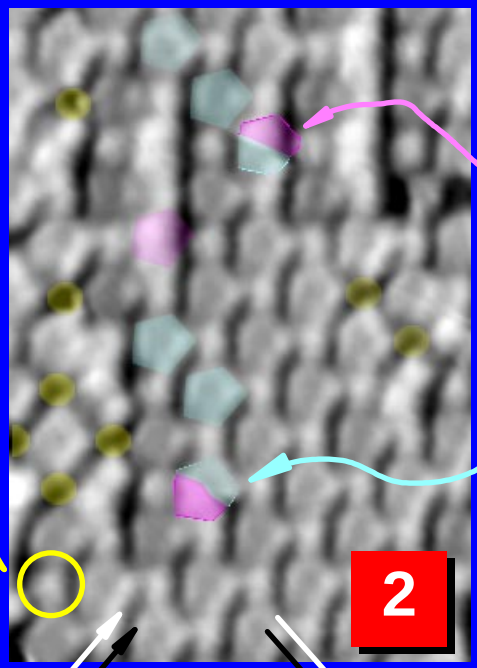
Filled States (2 V) 45 Å × 45 Å

[$\bar{1}$10]

Scan Direction

[33$\bar{2}$]

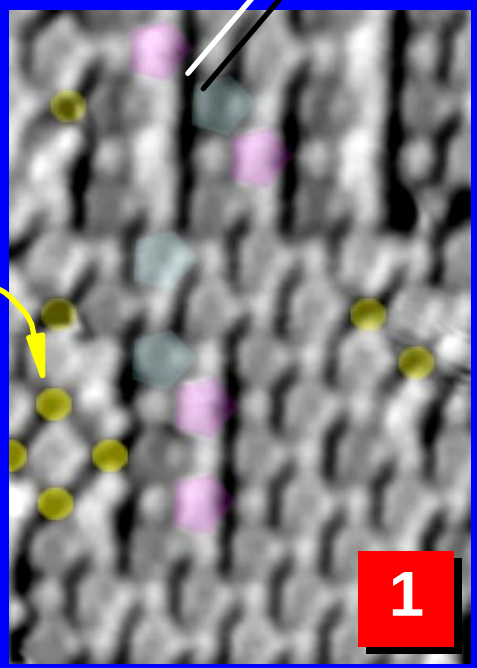
adatoms never hops

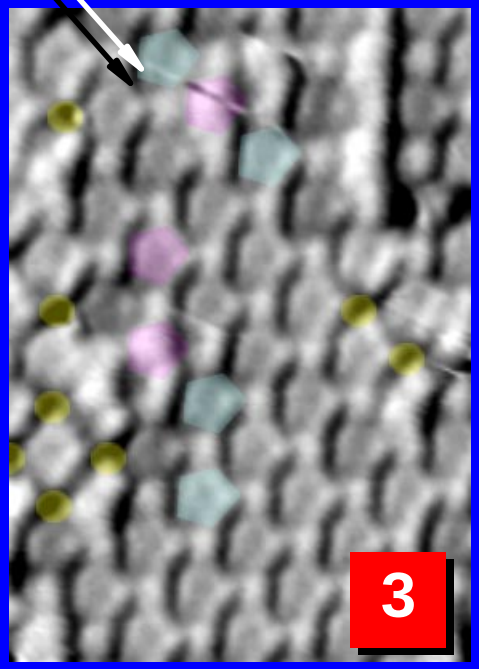


Interstitial hopped out between scans

Interstitial hopped in between scans

adatom vacancy defect





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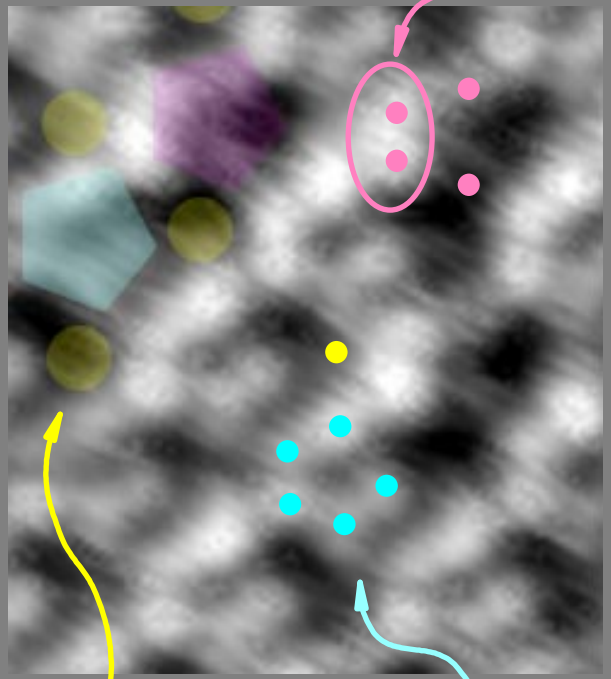
Filled and empty states STM images

Empty States (1.5 V)

bright dimer on regular tetramer

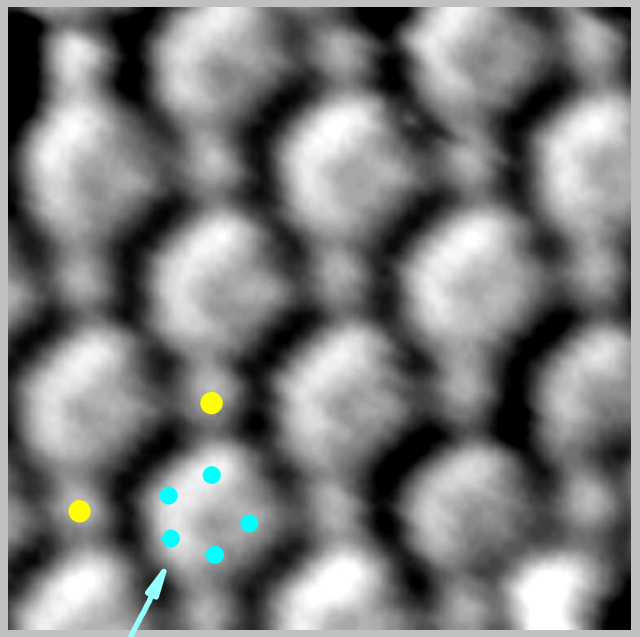


adatom looks dark

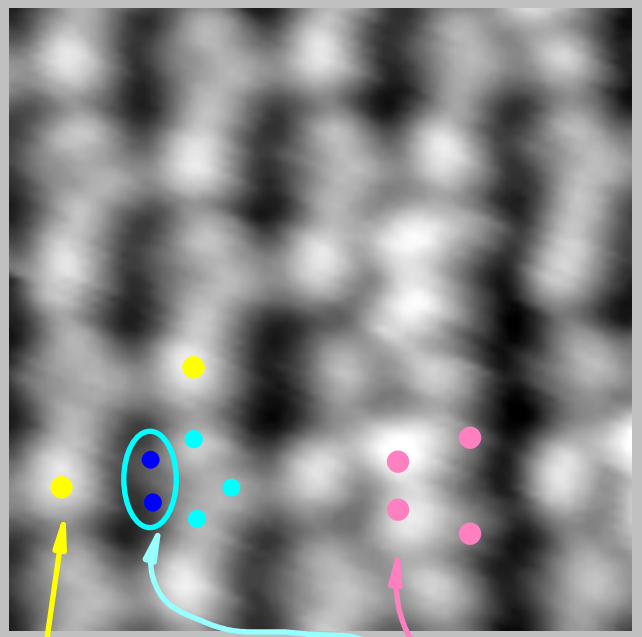
interstitial pentamer looks flat

Filled States Bias Dependence

(2.2 V)



(1.6 V)



interstitial pentamer brighter than adatom, and buckled

adatoms brighter than interstitial

dimer on interstitial pentamer looks dark

tetramer brightness is independent of bias

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The origins of self-interstitials

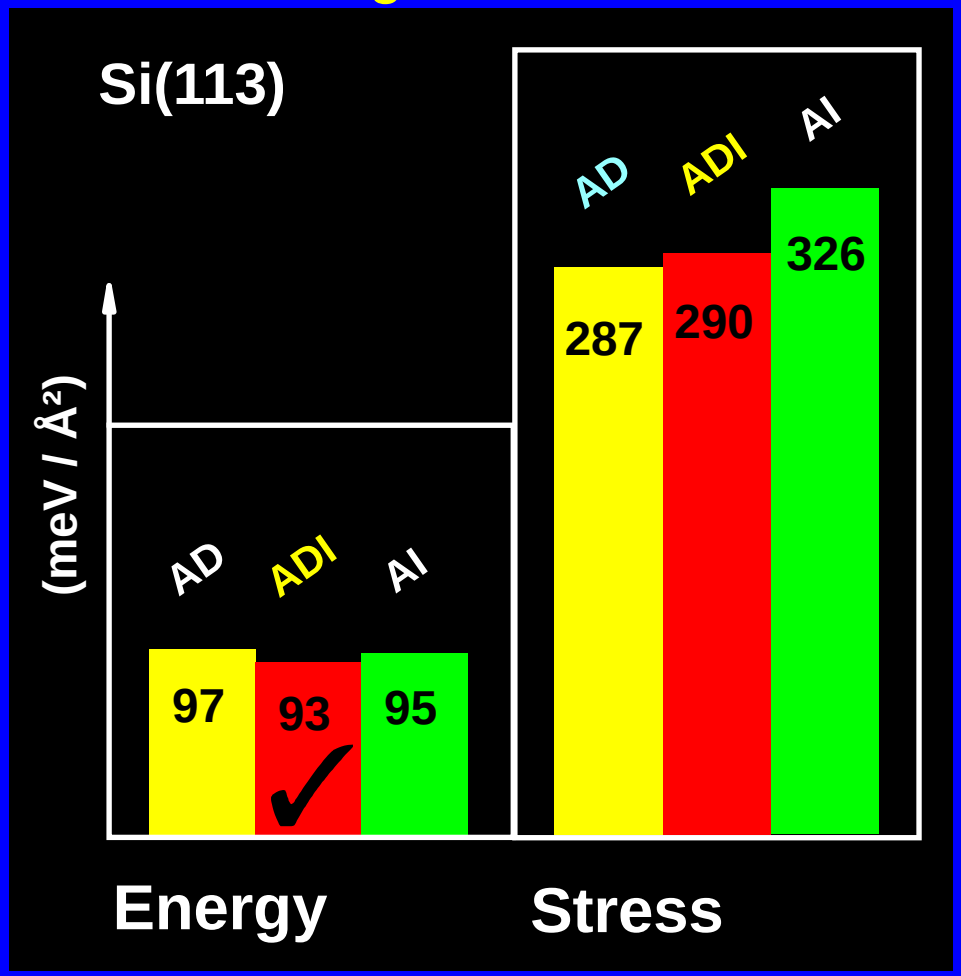
Relieve tensile surface stress?

- Compute surface stresses with LDA.

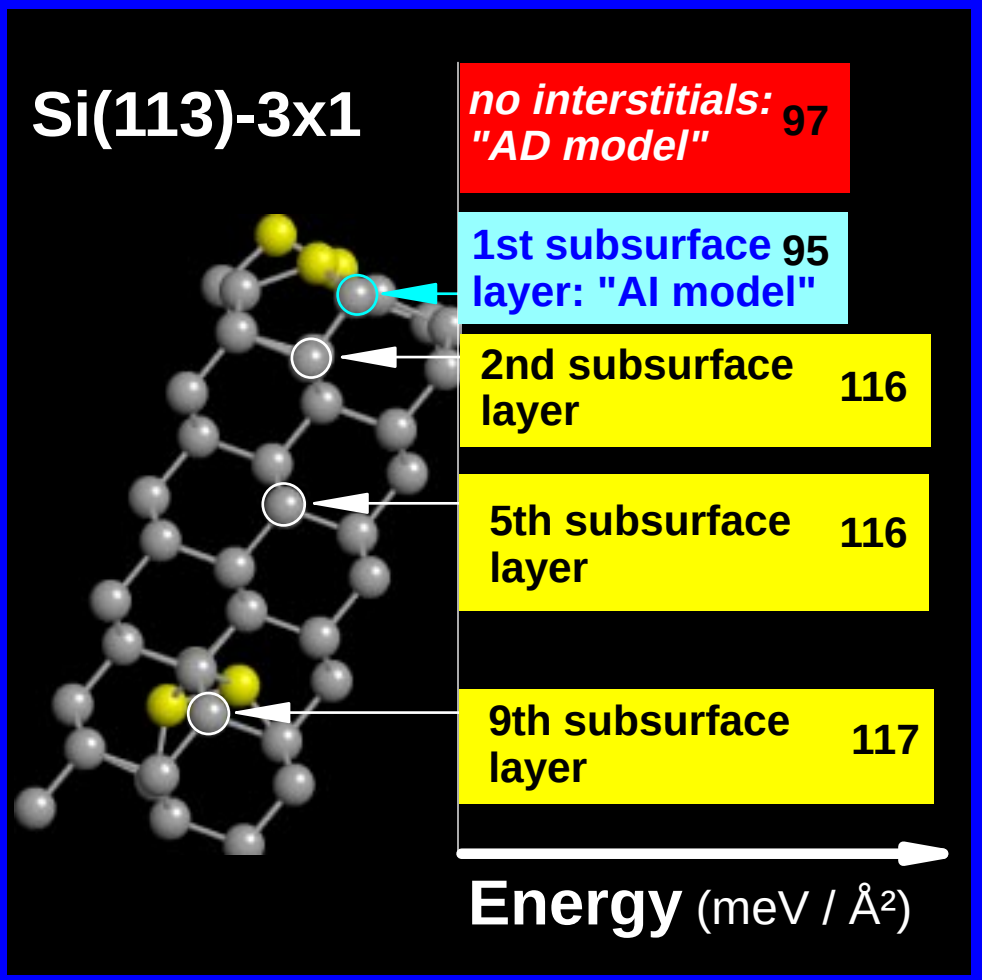
Diffuse out from the bulk?

- Use LDA to calculate energy vs. distance away from the surface.

Surface energies and stresses



The cost of subsurface interstitials



Comments and conclusions

Why is the Si Adatom-Interstitial-Dimer reconstruction so stable?

- "Relief of tensile surface stress" (Dabrowski, PRL '94)
  - Calculated energies of deep interstitials: no supporting evidence
  - Calculated surface stresses: no supporting evidence

What is the nature of the Ge(113)-3x1/3x2 surface?

- "SXRD: random 50±10% distribution of subsurface interstitials" (Vogler, PRB '98)
  - STM: 50% coexistence of small AID and AI domains ($\Rightarrow$ 75% interstitials)
- STM: interstitial migrations $\Rightarrow$ 3x2 AID $\leftrightarrow$ 3x1 AI (Gai, PRB '97)
  - Theory: migration into bulk unlikely $\Rightarrow$ surface adsorbate gas?

Why does Ge support both AID and AI reconstructions?

- "3x2 AID reconstruction $\Rightarrow$ doubly occupied surface band" (Dabrowski)
  - Additional interstitial (3x2 AID $\rightarrow$ 3x1 AI) dopes conduction bands
  - Si gap > Ge gap $\Rightarrow$ Si-3x2 (AID), Ge-3x2/3x1 (AID/AI)