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Computational Engineering of the Stability and Optical Gaps of SiC Quantum Dots

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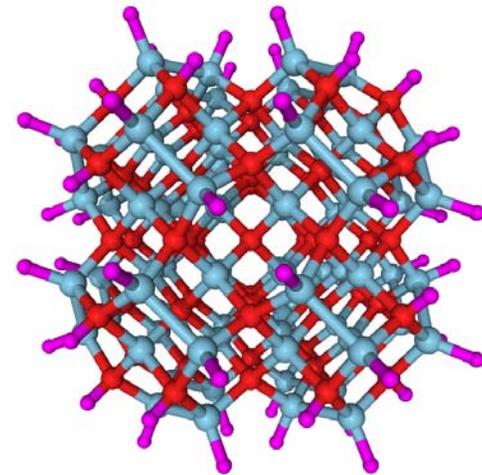
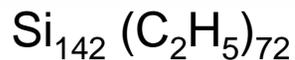
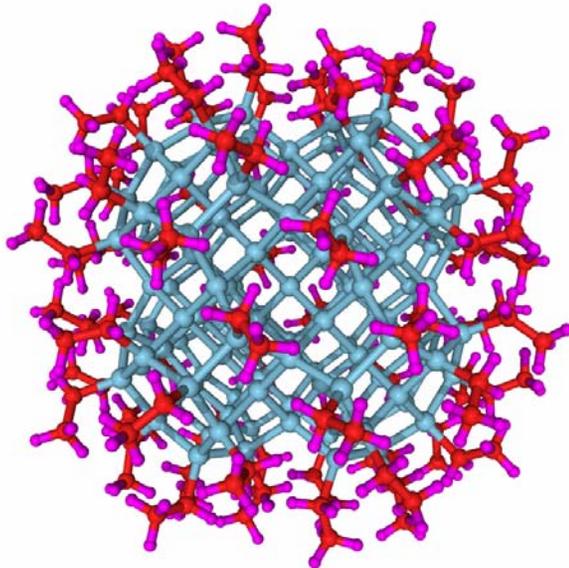
Computational engineering of the stability and optical gaps of SiC quantum dots

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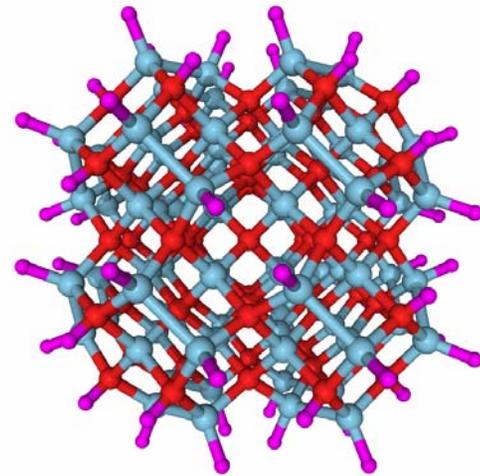
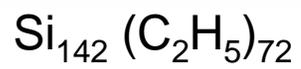
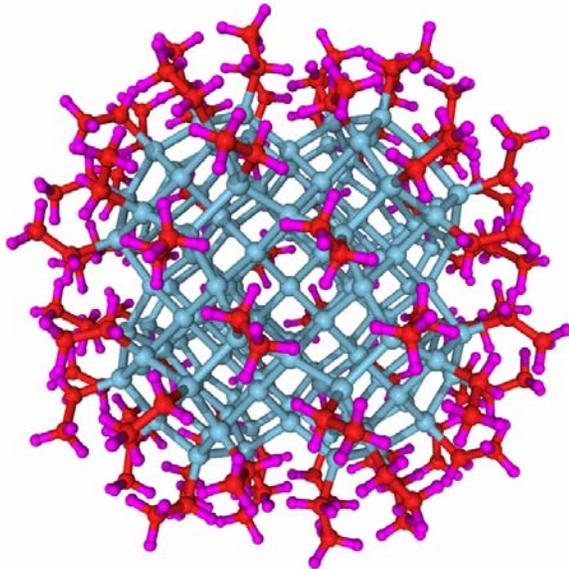
[§]Université de Poitiers, Cedex France

Si ●
C ●
H ●



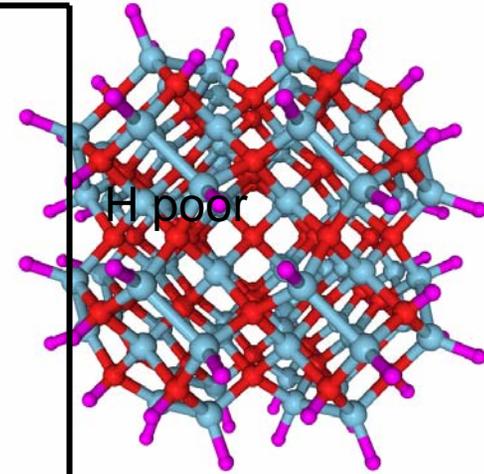
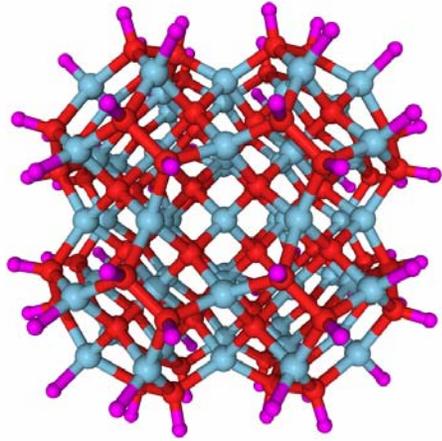
Why SiC quantum dots?

Si ●
C ●
H ●



Different Surface structures

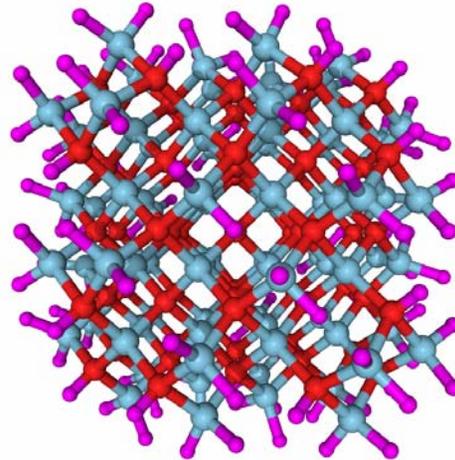
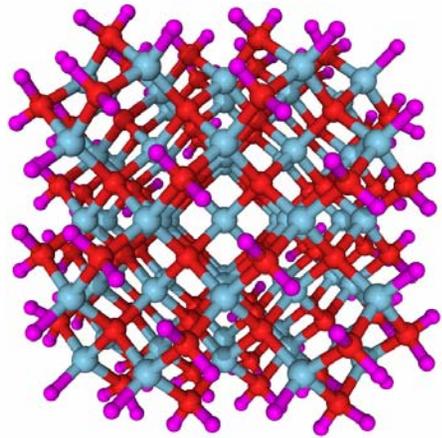
Reconstructed



H poor



Un-reconstructed



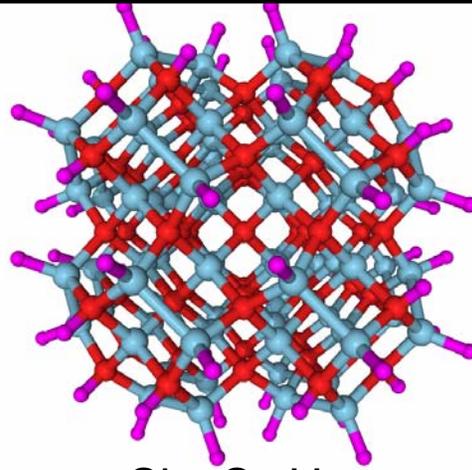
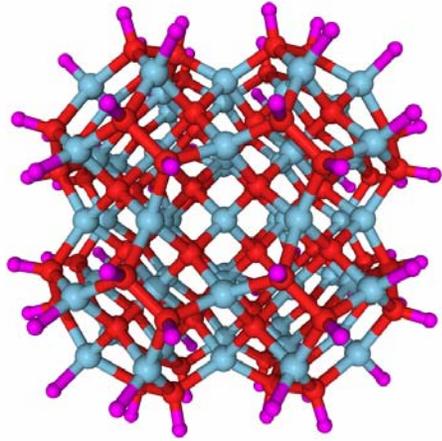
H rich

C-term

Si-term

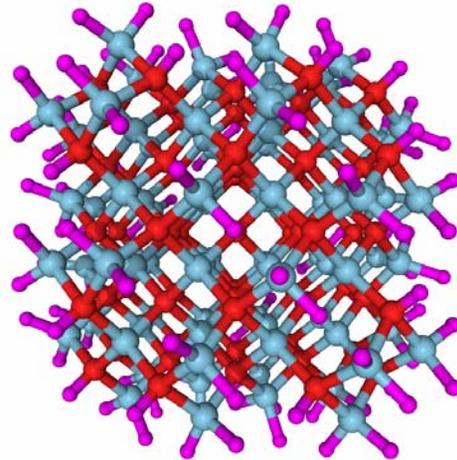
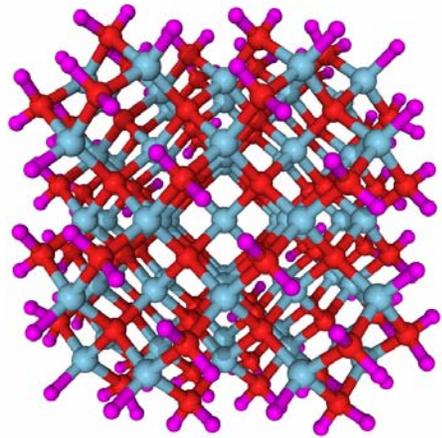
Different Surface structures

Reconstructed



H poor

Un-reconstructed

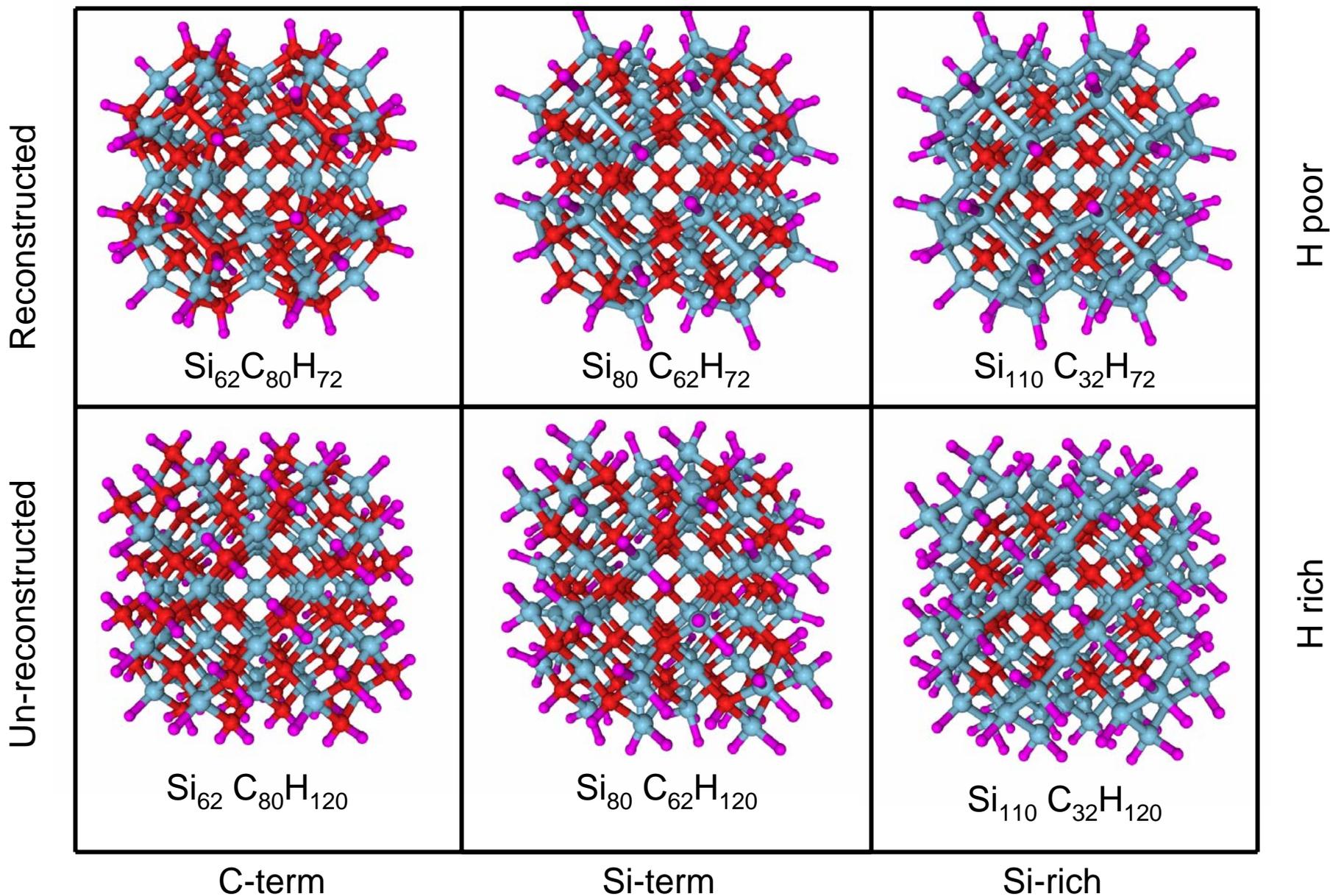


H rich

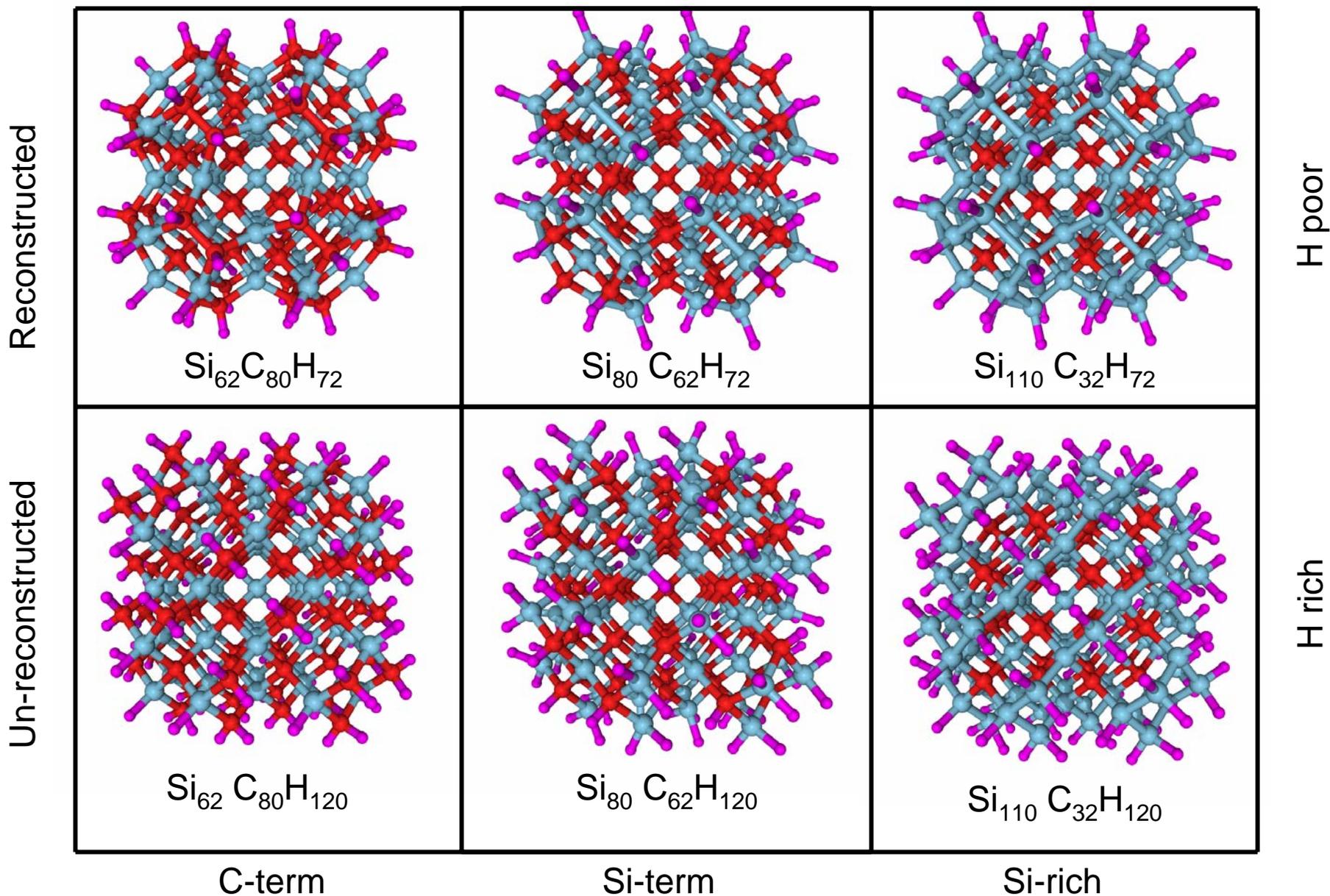
C-term

Si-term

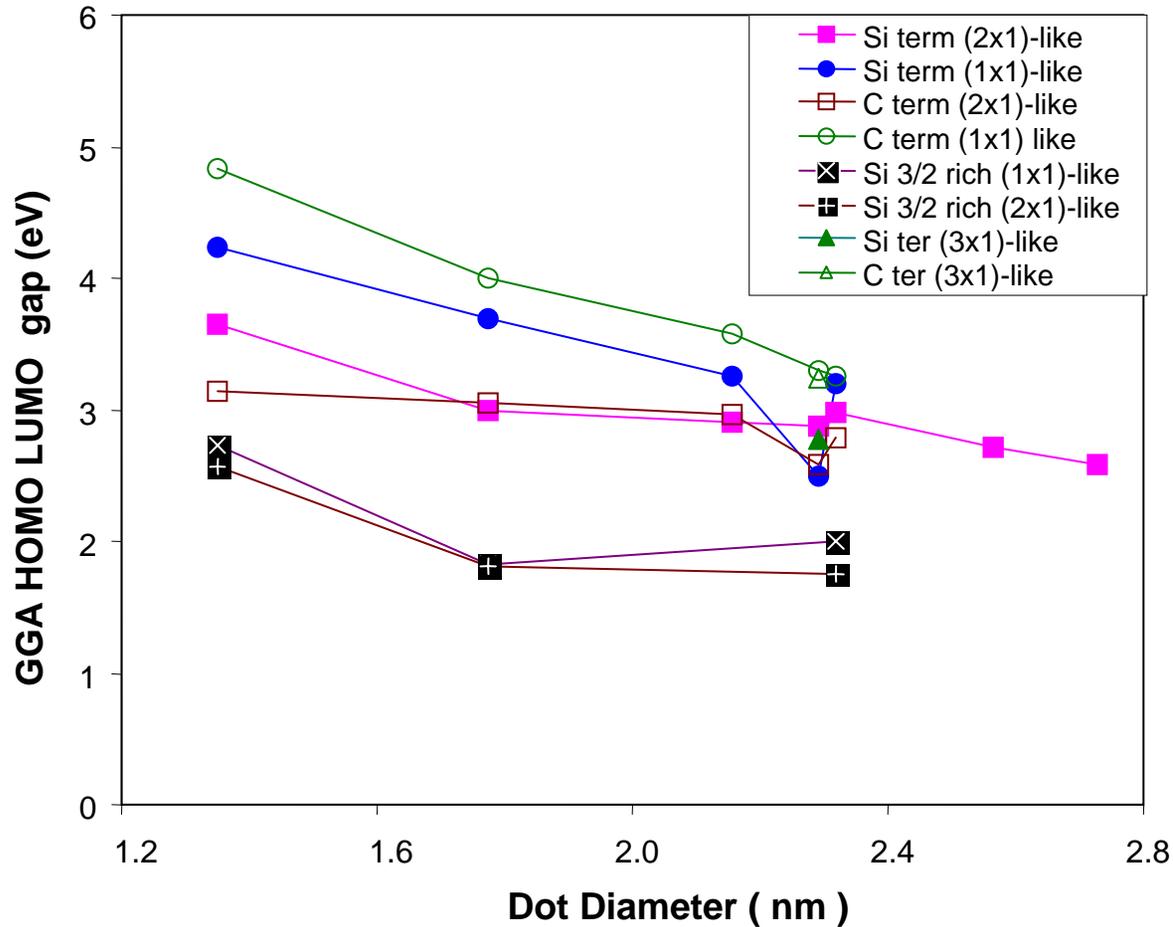
Different Surface structures



Size dependence for all this structures!

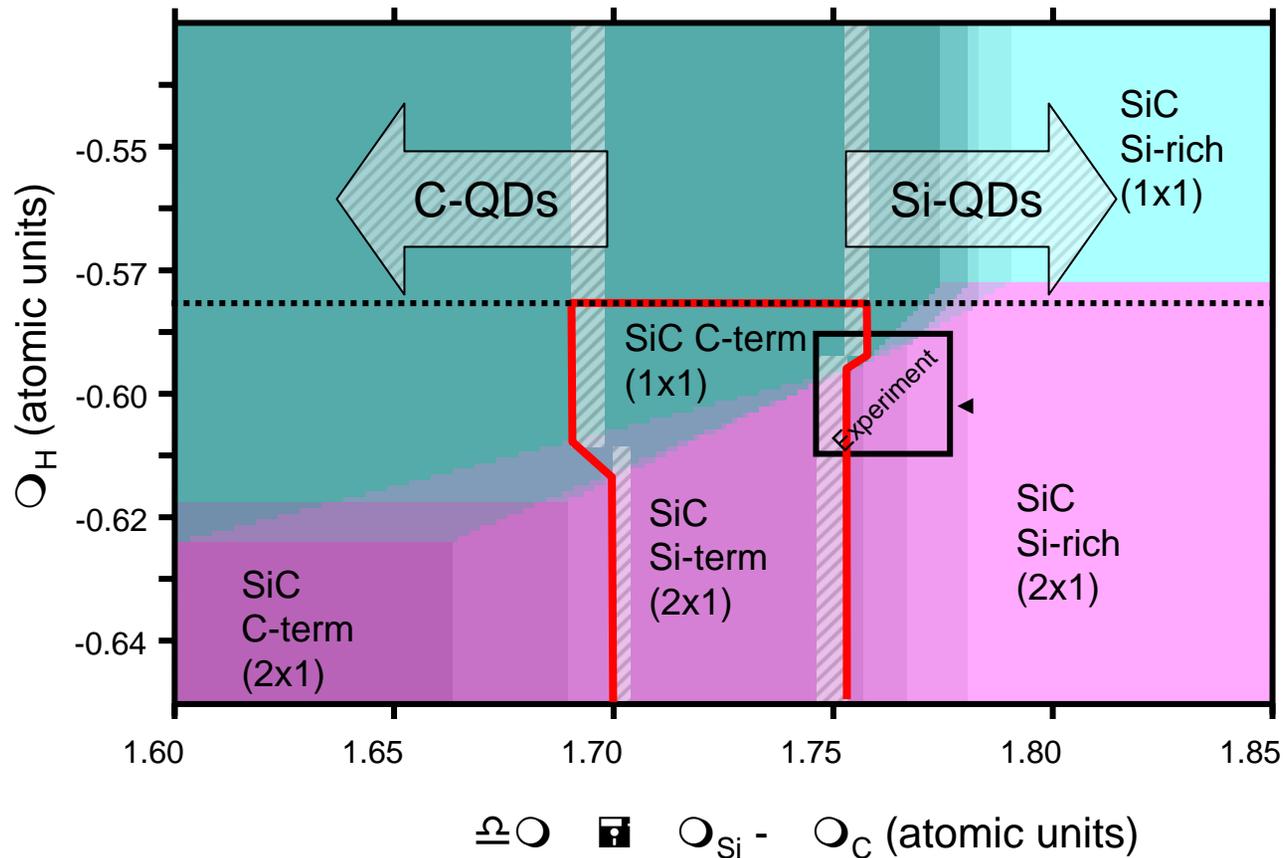


Single particle gap of SiC QD as a function of size and surface structure



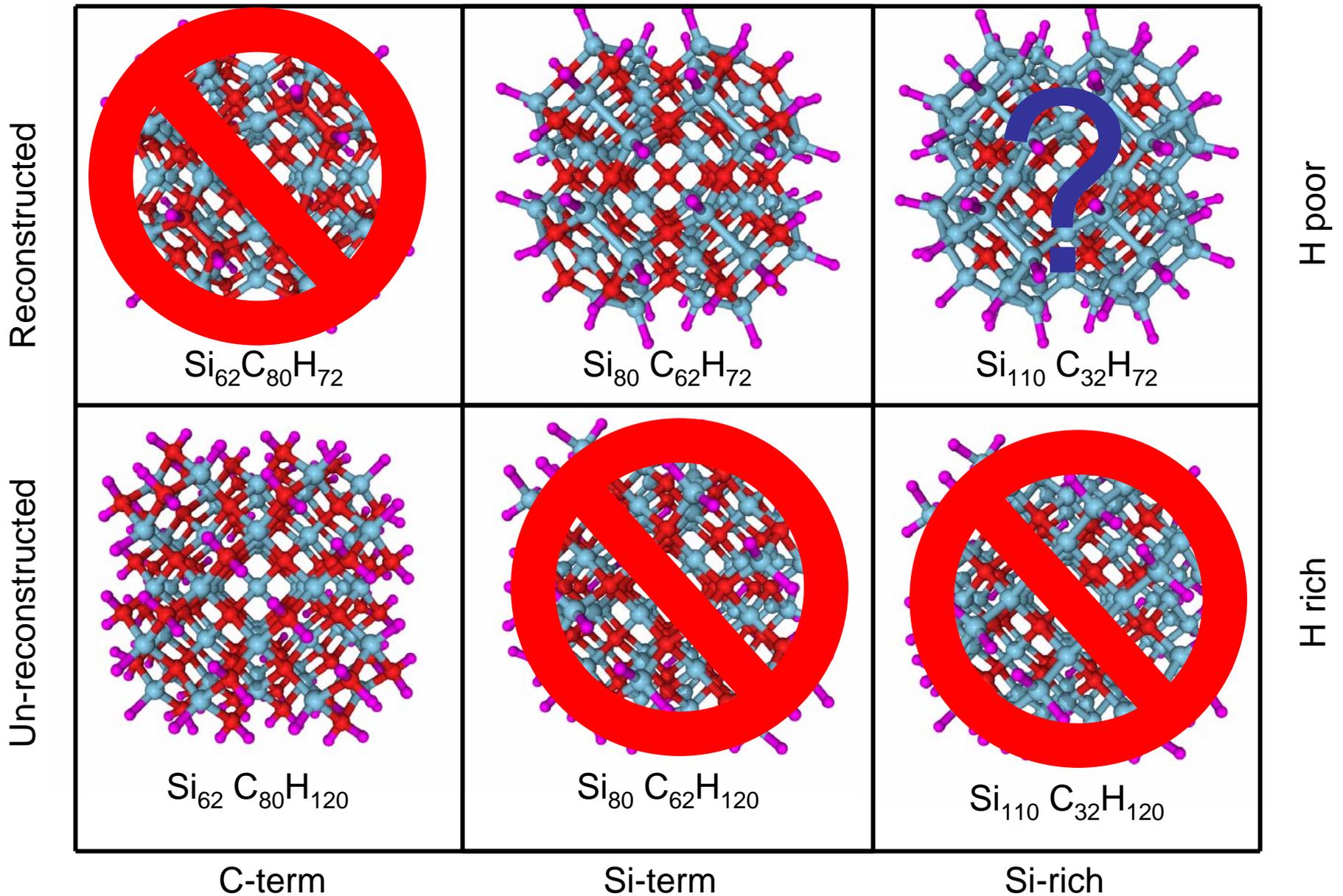
The surface structure is as important as the size as a determiner of the gap

SiC QDs: Surface phase diagram under equilibrium

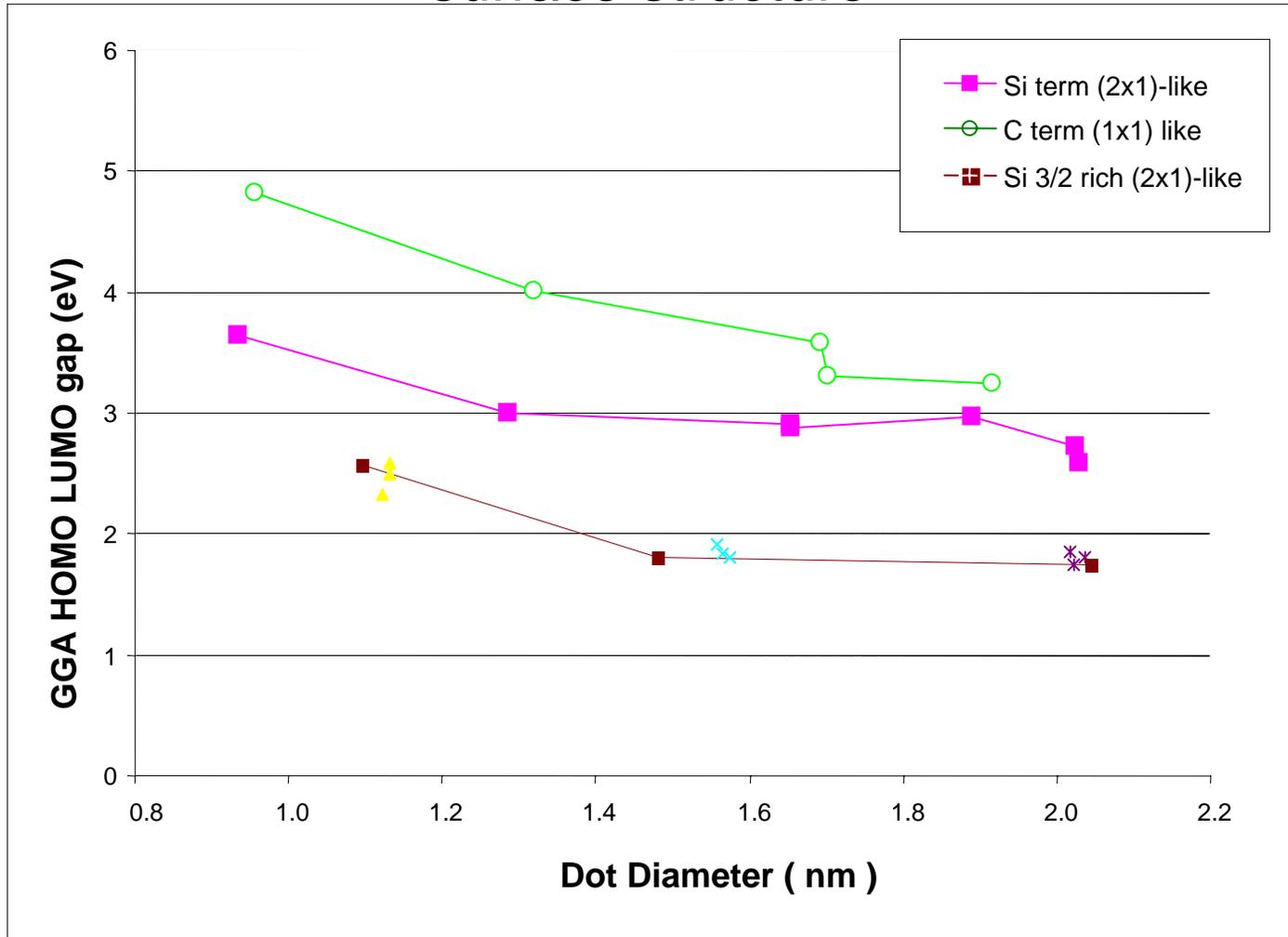


Only three types of surfaces are in principle possible at or near equilibrium.

Only two surfaces are stable



Single particle gap of SiC QDs as a function of size and surface structure

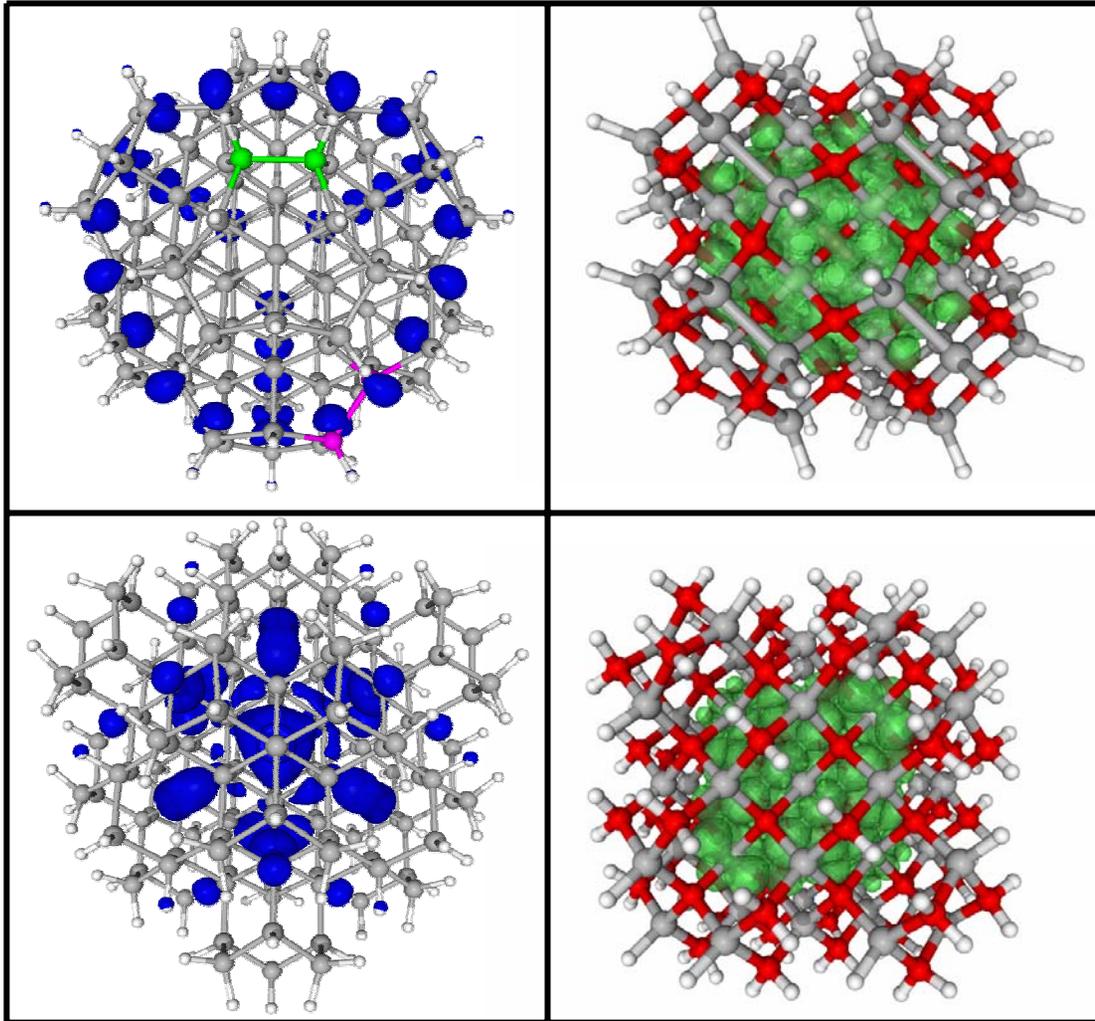


Only three types of surfaces are in principle possible near equilibrium.

Localization of band edge wave functions

Si Qdots

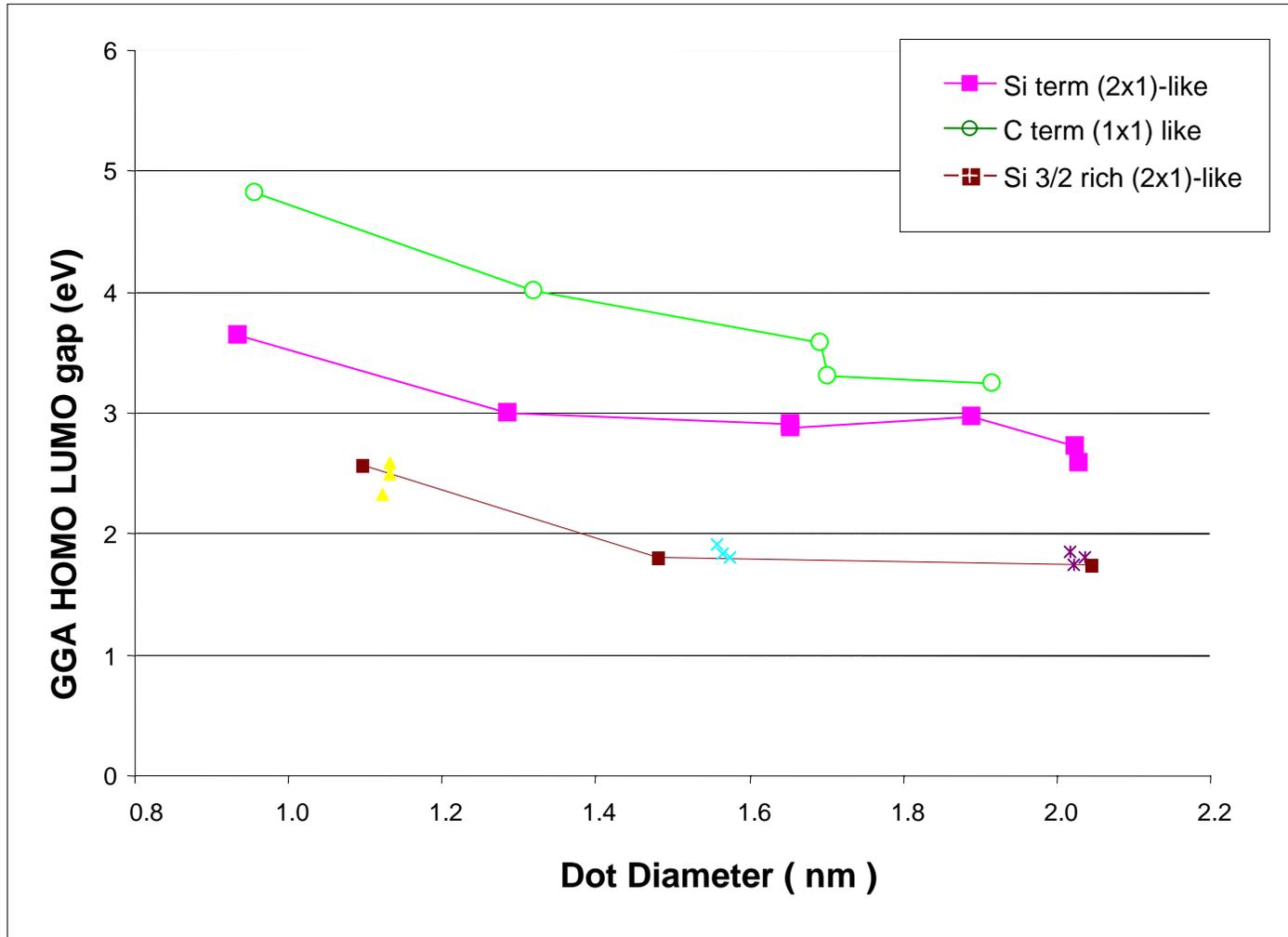
SiC Qdots

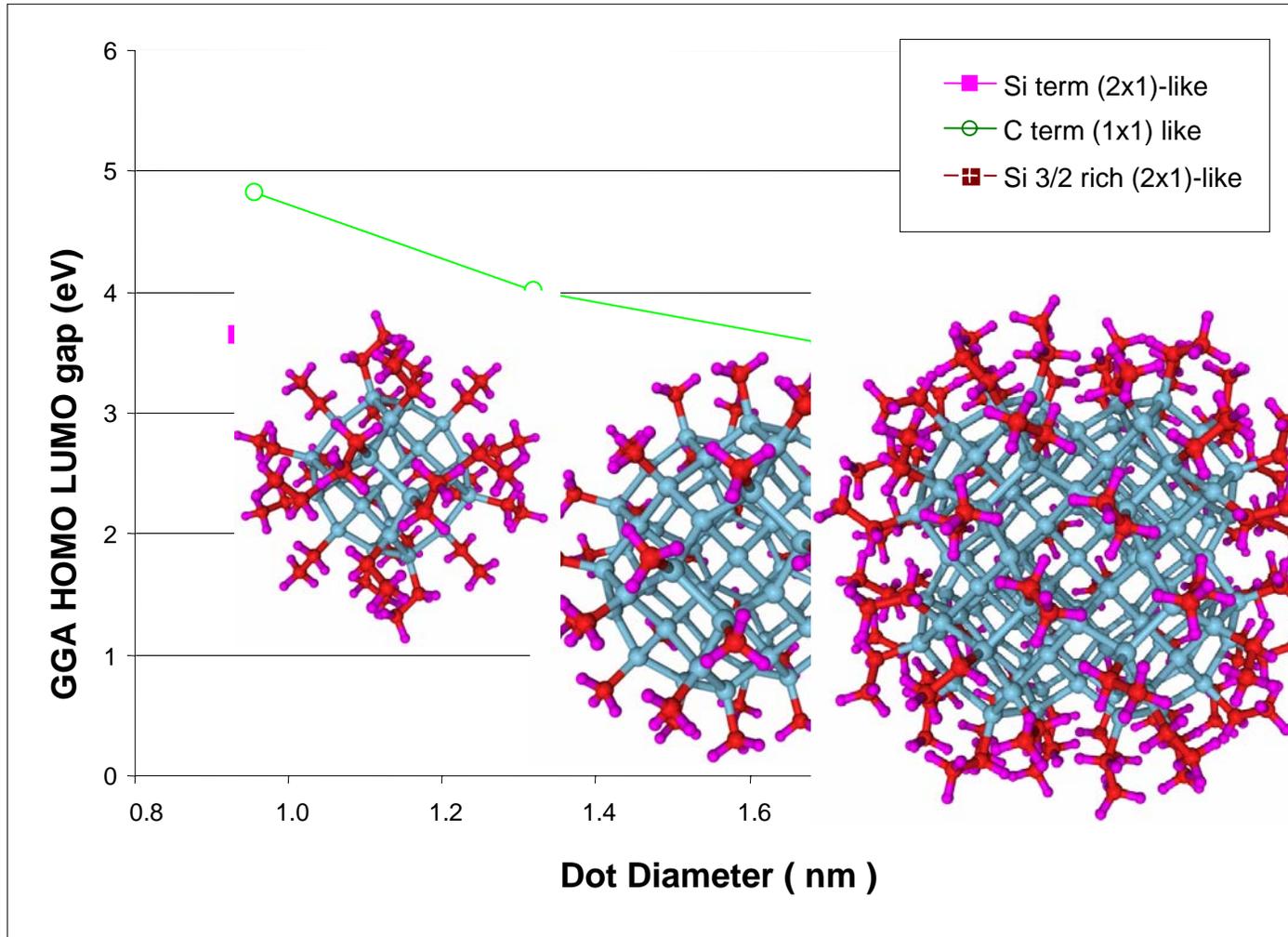


(Si-term reconstructed)

(C-term
Un -reconstructed)

In SiC surface-induced strain and not surface localization originate large gap differences





Conclusions

- In SiC QDs surface composition and structure are as important as size for the optical gap
- Two surfaces are possible near equilibrium; one is close
- Different experimental conditions quite different optical gaps
- C-term H-rich SiC QDs have the largest gaps in group IV
- Si-enriched SiC QDs have similar gaps than reconstructed alkyl terminated pure Si dots.

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