




LEED and Ab-Initio Study of the Si(111)3x2-Sm Reconstruction

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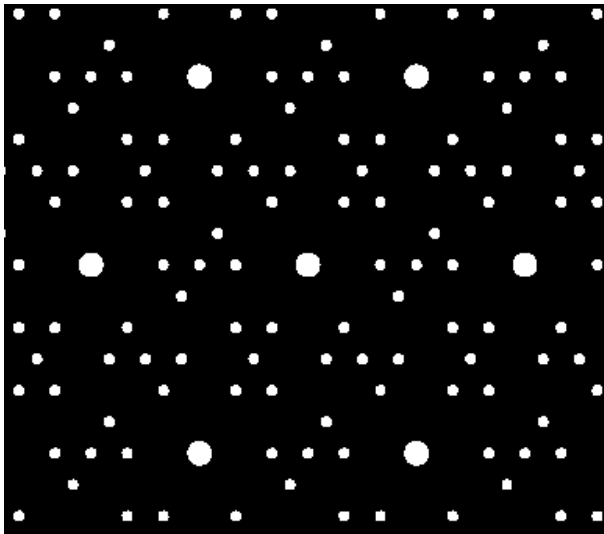
LEED and Ab-Initio Study of the Si(111)3x2-Sm Reconstruction

- The Si(111)3x2-Sm System
- Low Energy Electron Diffraction Results
- Comparison with Suggestions in the Literature
- DFT Ab-Initio Calculation using the CASTEP code
- Conclusions and Future work

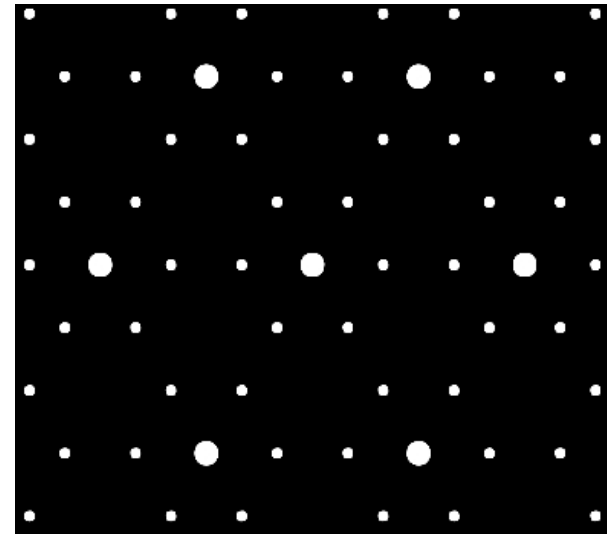
LEED-STM Discrepancy in Si(111)3x2-X Systems

- STM shows a 3x2 structure on the surface.
- LEED pattern is 3x1 – half order spots missing

Expected LEED Spot Patterns



3x2

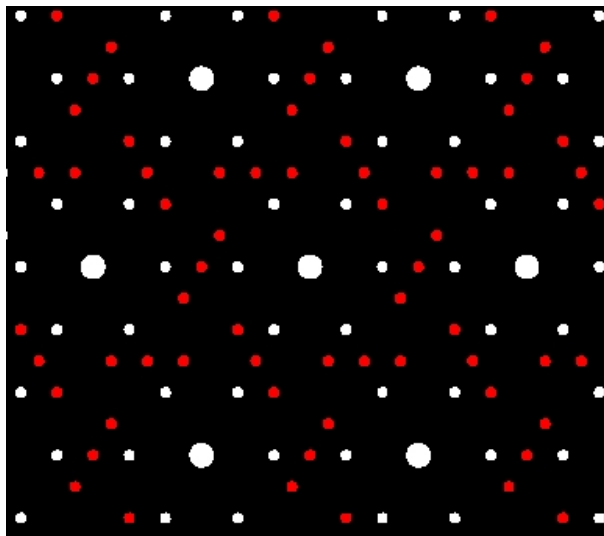


3x1

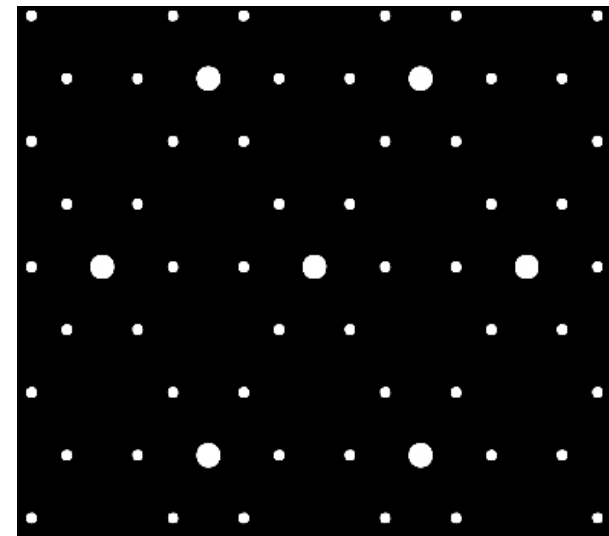
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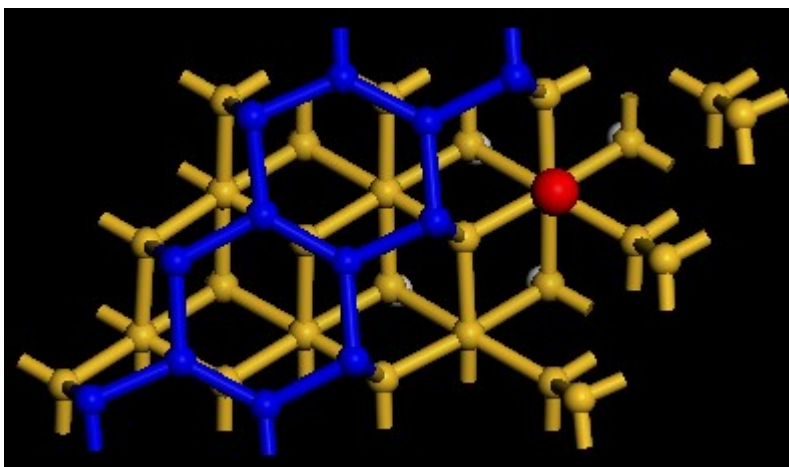


3x2

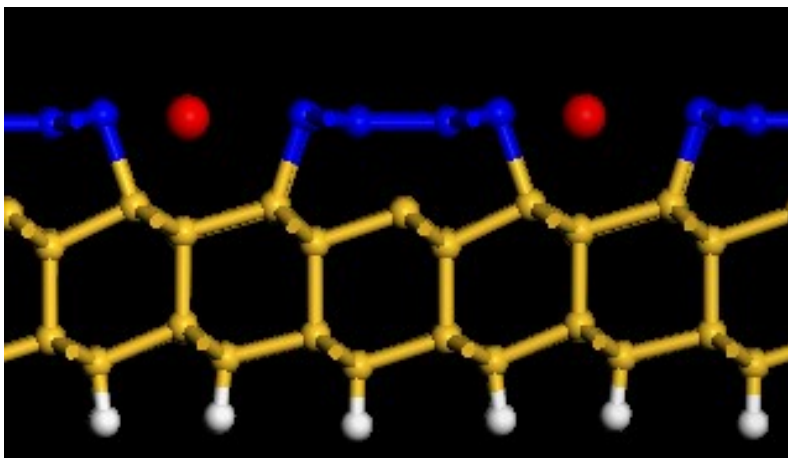


3x1

Structural Model and the Idea of Registry Shifts

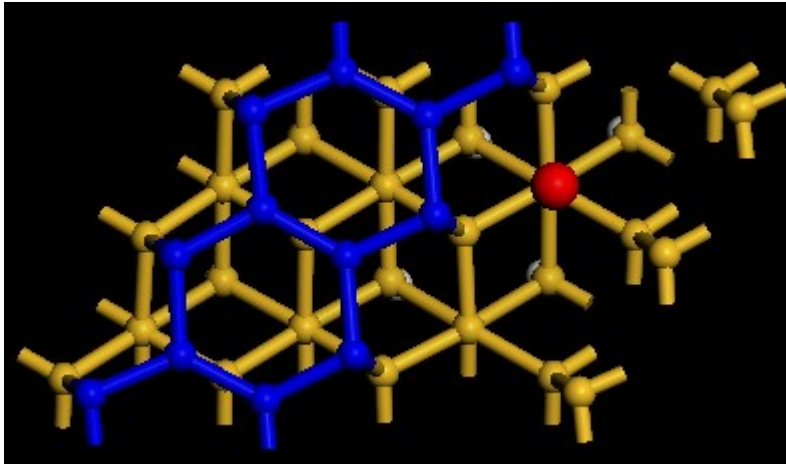


- VASP DFT Ab-Initio calculation
Phys. Rev. B., V67, (2003)
p195413, Palmino et al.
- Based on structure suggested
for Si(111) 3x2-Ba,
Phys. Rev. Lett., V87, (2001)
p56104, Lee et al.

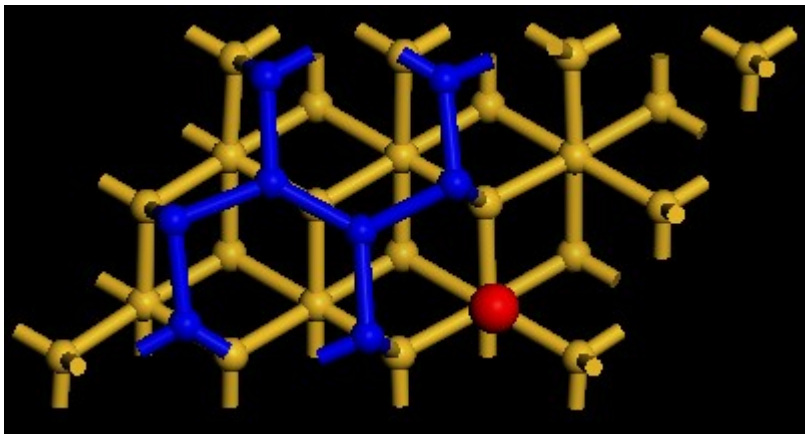


- Interference of amplitudes
from two registry shifted cells
proposed to explain
cancellation of x2 spots
- Quantitative calculation in
literature Phys. Rev. B., V67,
(2003), p85411, Schafer et al.

Structural Model and the Idea of Registry Shifts

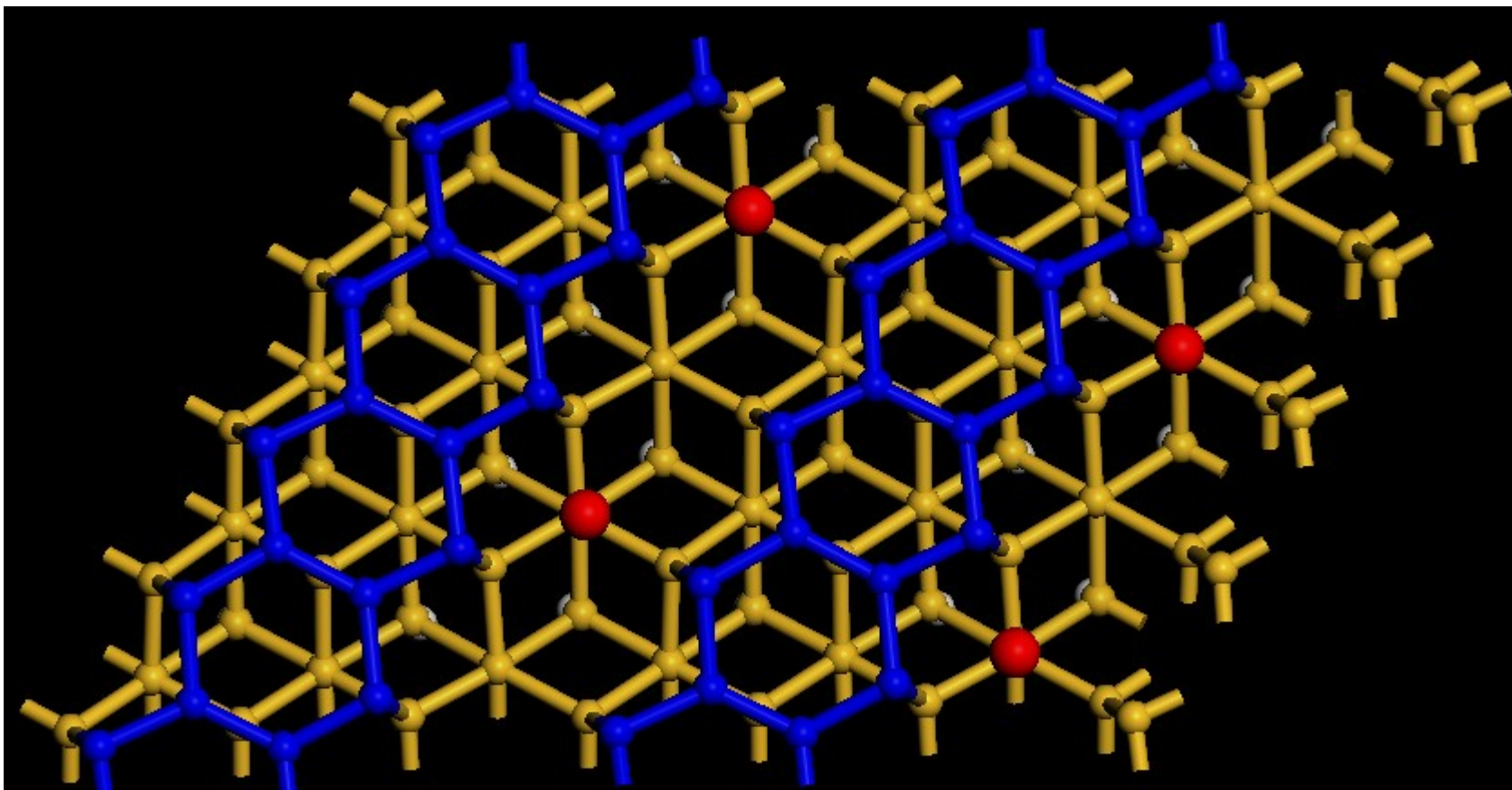


- VASP DFT Ab-Initio calculation
- Based on structure suggested for Si(111) 3x2-Ba
- Phys. Rev. B., V48, (1993) p11014-11021, Wigren et al.



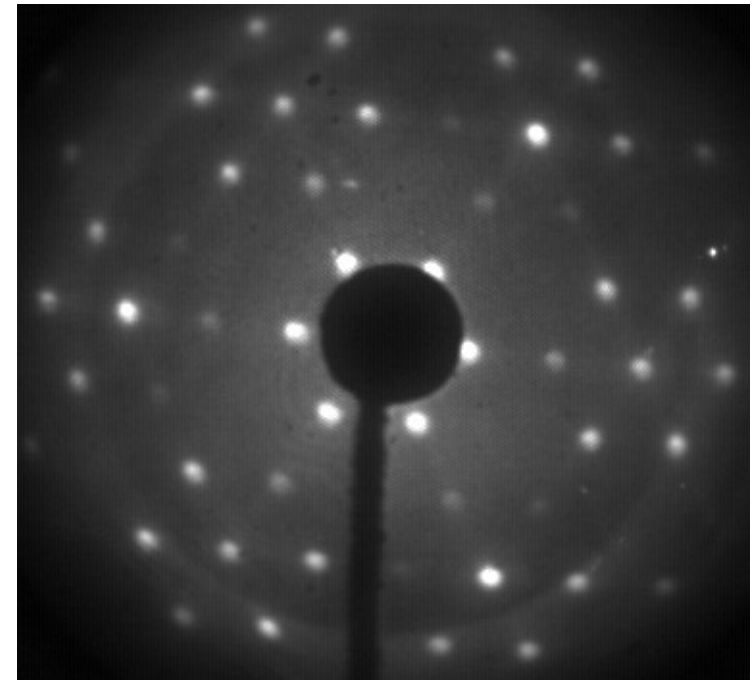
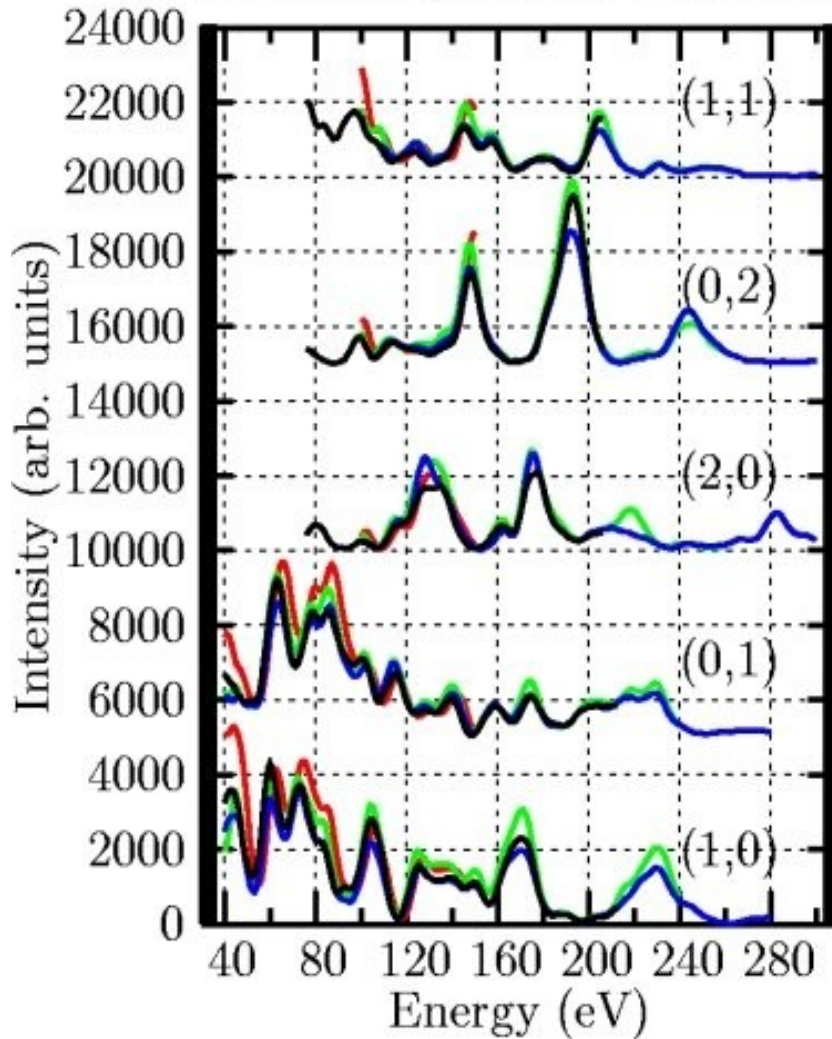
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Structural Model and the Idea of Registry Shifts



Low Energy Electron Diffraction Curves

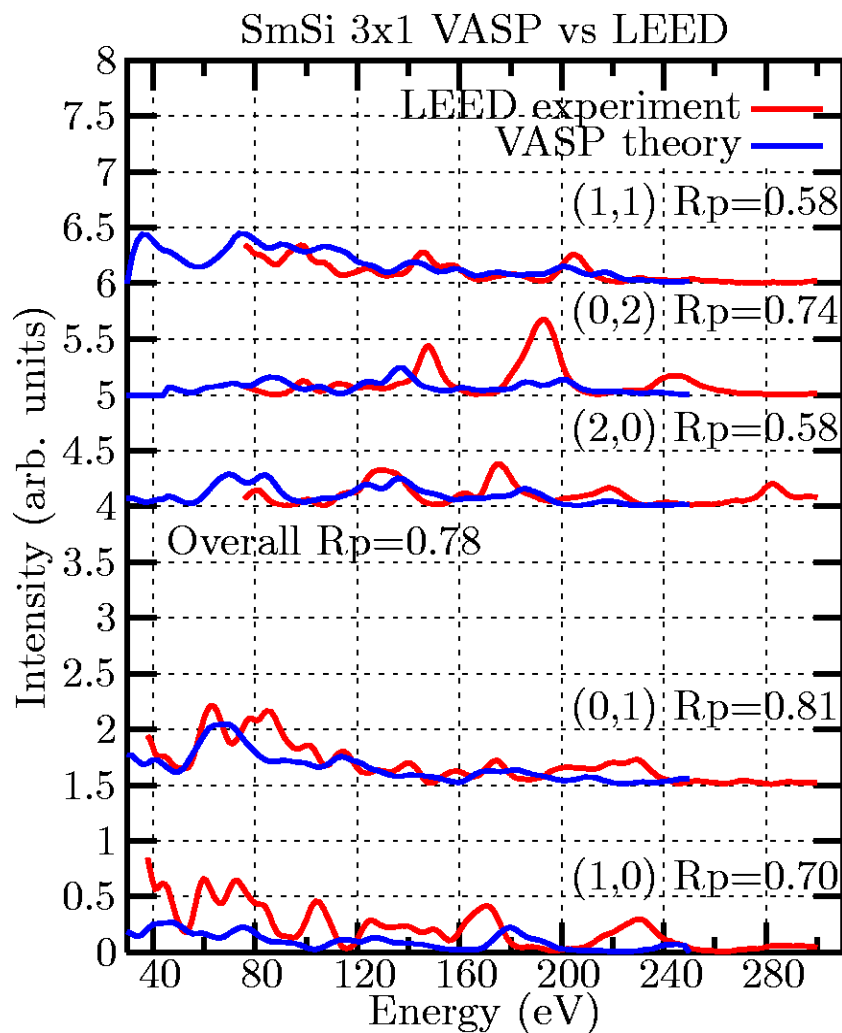
SmSi 3x1 Integer Spots Experimental



LEED image 46eV

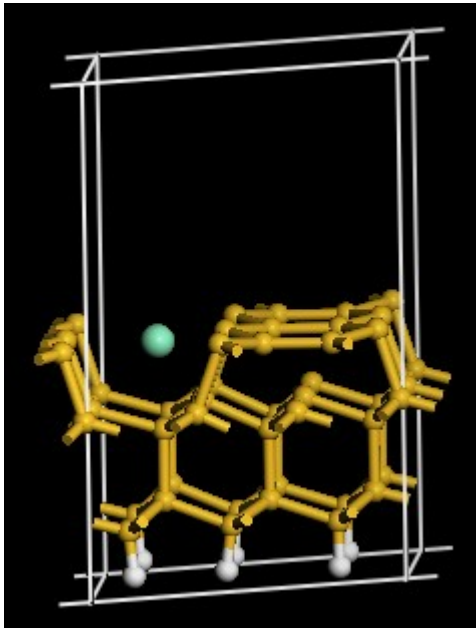
- Deposit 1ML Sm on clean Si(111)
- Anneal 300 °C 15 mins
- Clean, thermally resilient structure

Theory-Experiment Pendry R-Factor Comparison



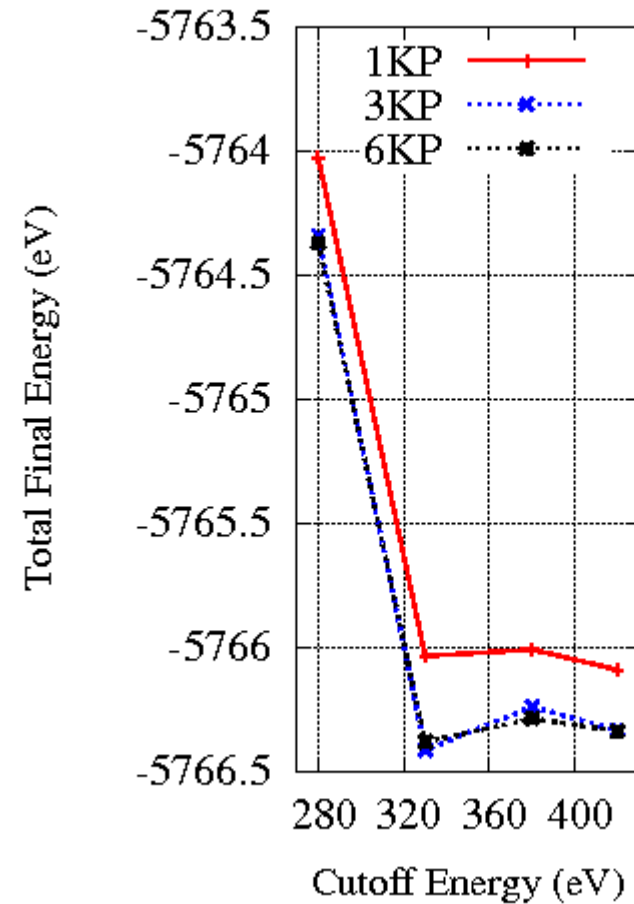
- Pendry R-Factors calculated using the CAVLEED program
- Overall R-Factor is 0.78
- Good is <0.5
- Acceptable is <0.6
- Poor R-Factors when compared to LEED I(V)
- Where next?

Ab-Initio Calculation using CASTEP

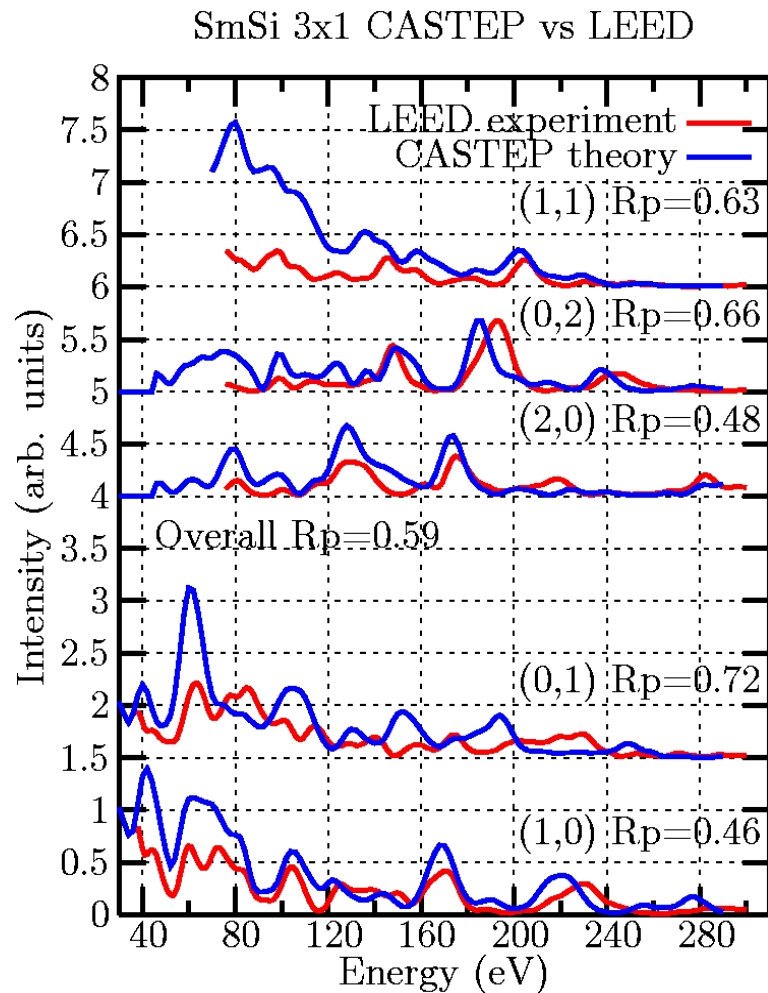


- CASTEP Ab-Initio DFT code
- Full basis set convergence
- Structure relaxation performed on 32 cpus of HPCx
- Main relaxation in spacing from layer 1 to layer 2

SmSi Supercell k-point and Cutoff Convergence



CASTEP vs LEED Experiment R-Factor Comparison



- Overall Pendry R-Factor improved to below 0.6 without any smoothing
- Main discrepancy in x2 scattered spots
- Problems elsewhere at high energy

Conclusions and Future Work

- DFT and LEED have been shown to qualitatively explain the STM-LEED discrepancy observed for the Si(111)3x2-Sm Structure.
- A Pendry R-Factor comparison has shown that a structure with a relaxed top honeycomb layer agrees better with LEED I(V) than the VASP result.
- Investigate why the R-Factors for spot groups with a contribution from the x2 direction are consistently worse.

Acknowledgements.

- Supervisors; Matt Probert (theory) Steve Tear (Experiment)
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- Travel Bursaries; CR Barber Trust, IoP Thin Films and Surfaces