Investigating Preservation of Local Structure in 2-D $Re_6Se_8Cl_2$ After Surface Functionalization

Using PDF to Characterize Local Structure Behavior in Surface Functionalized 2-D Materials

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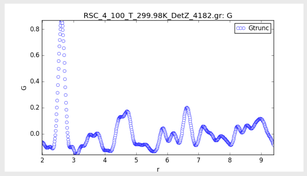
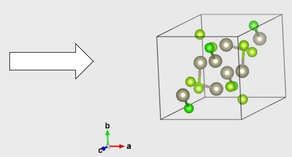
INTRODUCTION

- 2-D materials are promising candidates for a multitude of next-generation technologies.
- Surface functionalization allows the surface chemistry and, subsequently, the properties, of a 2-dimensional material to be modified according to the demand of a particular application.
- A major drawback of surface functionalization is that, in the process of functionalizing such materials, the integrity of the internal structure (layer alignment and spacing) is compromised.
- Herein, we investigate the preservation of local structure in 2-D $Re_6Se_8Cl_2$, a well-ordered transition-metal dichalcogenide, after surface functionalization and heating to high temperatures.

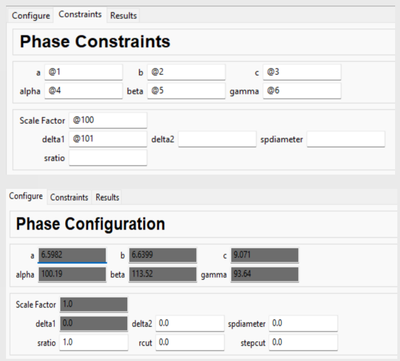
METHODOLOGY



$Re_6Se_8Cl_2$ low r PDF

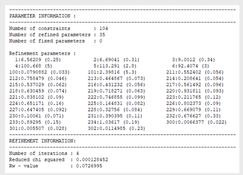


$Re_6Se_8Cl_2$ structural model in VESTA

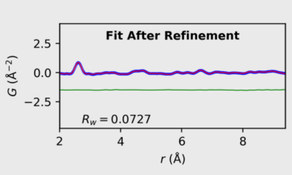


Constraining model variables as fixed parameters in PDFgui

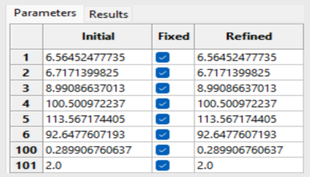
Constrained variables (lattice parameters, sale factor, etc.)



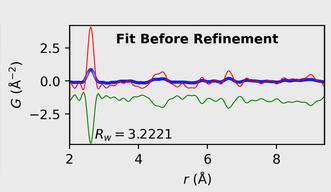
Fit summary output file



Refined PDF fit



Refinement parameters



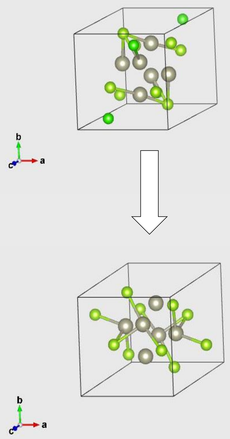
Unrefined $Re_6Se_8Cl_2$ PDF

CONCLUSIONS/FUTURE GOALS

- Conclusions:
  - Local structure preserved in Re6Se8 following functionalization, although alignment and spacing of layers was compromised.
  - At ~400K, the material undergoes a phase transition, accompanied by abrupt changes in atomic positions and unit cell parameters.
- Future Goals:
  - Investigate and characterize phase transition using PDF modelling.
  - Determine effect of phase transition on material properties and performance.

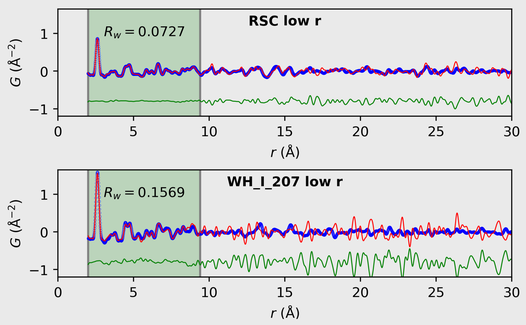
RESULTS

Is local structure preserved after surface functionalization?



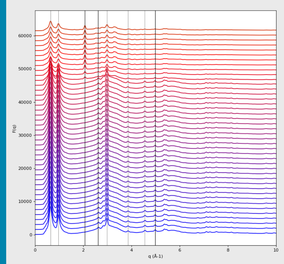
Pristine VESTA structure (top) and functionalized VESTA structure (bottom)

Short-range order (r=2-9.4) in $Re_6Se_8Cl_2$ (RSC) preserved in Re_6Se_8 (WH_I_207), demonstrating how the local structure is maintained after surface functionalization.



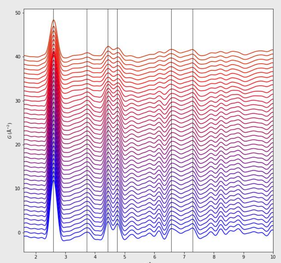
Pristine $Re_6Se_8Cl_2$ PDF fit (top) and functionalized PDF fit (bottom)

Is local structure preserved as temperature increases?



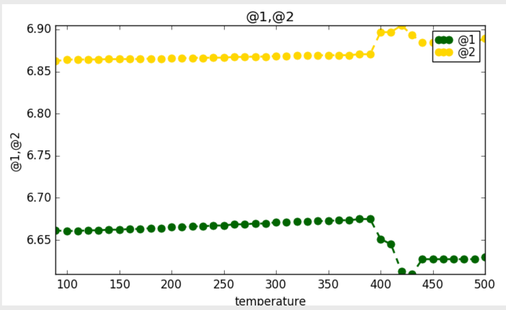
$Re_6Se_8Cl_2$ T-series F(Q)

*T_{min}– 89K(blue)
T_{max}– 500K(red)



$Re_6Se_8Cl_2$ T-series PDF

Around 400K, a peak emerges in the F(Q) and the lattice parameters fluctuate before settling at a new value. However, the PDF remains qualitatively unchanged.



Lattice parameters of functionalized material during heating

Acknowledgements

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