# Finding Negative Vacancy Formation Energies in Amorphous Silicon

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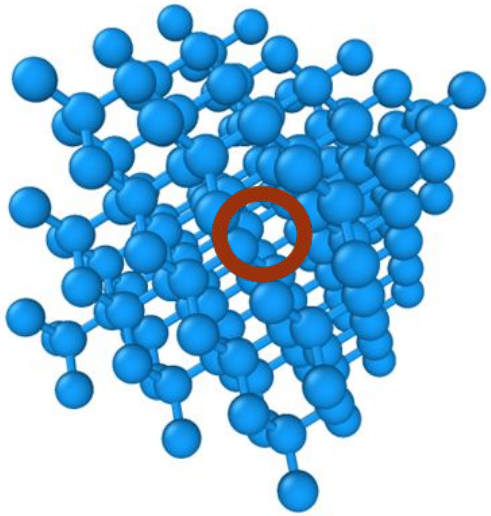
# Introduction

- Goal: determine whether Amorphous Silicon has negative vacancy formation energies.
- Vacancies control diffusion in solids
- Vacancy formation energies
- Amorphous solids



# Methodology

- Using LAMMPS software to conduct atomic simulations of amorphous silicon structures
- ADA Cluster at Texas A&M HPRC
- 20 cores with 2560 MB for between 20 and 100 Hrs.

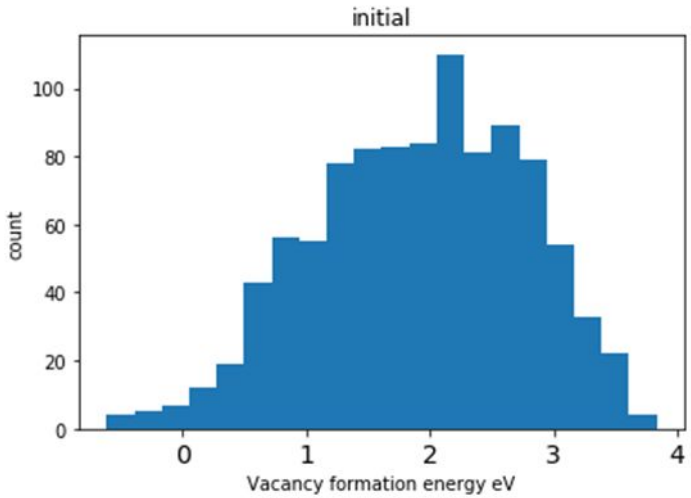
# Project Overview

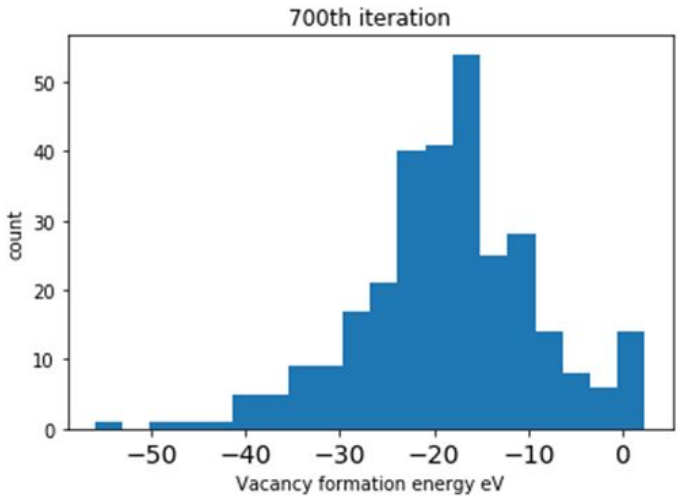
1. Melt and quench simulations
2. Preliminary vacancy formation energy calculation
3. Generalized atom removal energy calculations
4. Repeated calculations for varied simulation size
5. Self Interstitial formation energy calculations

# Results

- Vacancy Formation Energy Histograms

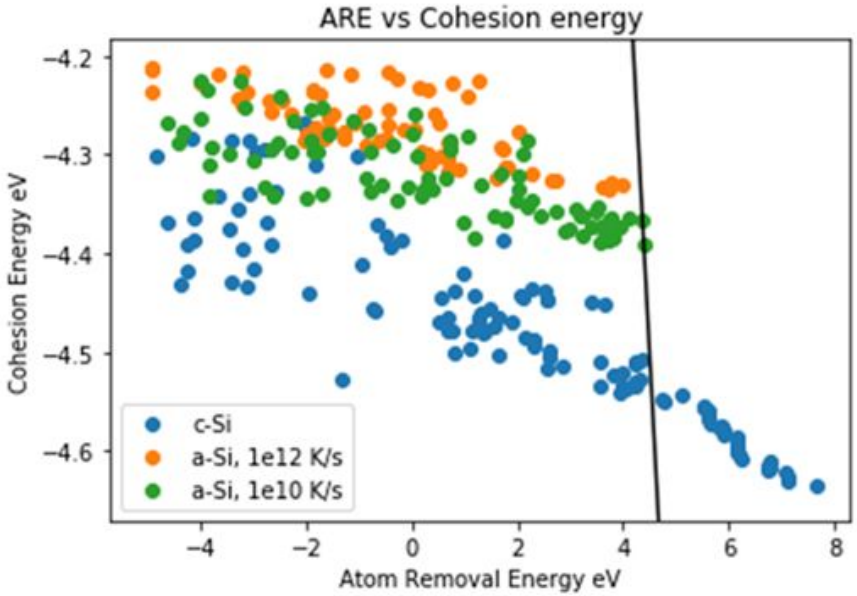
Performing algorithm on a-Si structures of 1000 atoms cooled at rates of 10^10 and 10^12K/s.



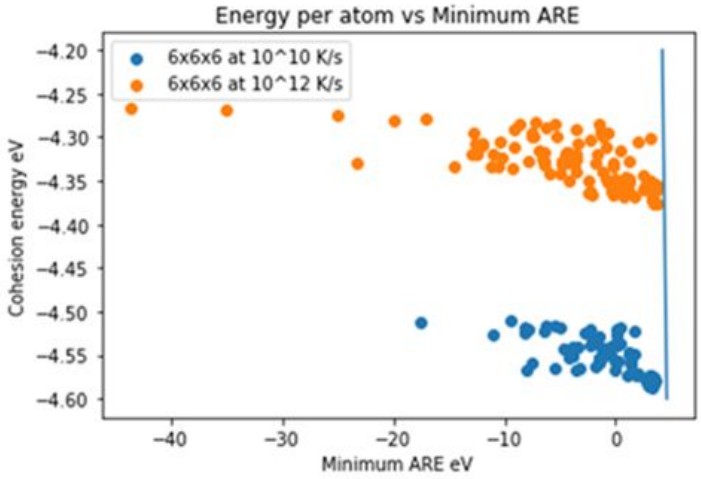
# Results

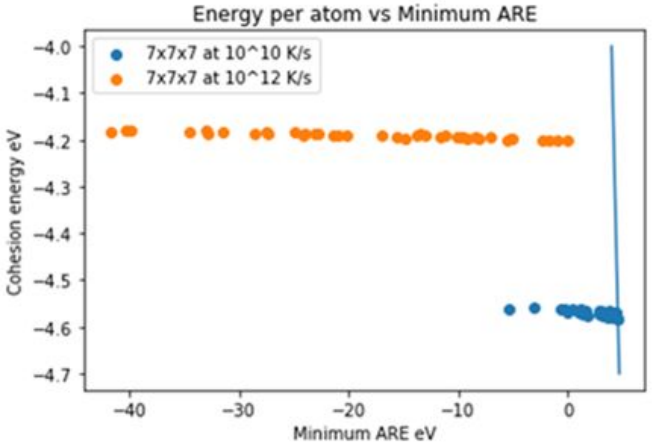
- Atom removal Energy vs Atom Cohesion Energy



# Results

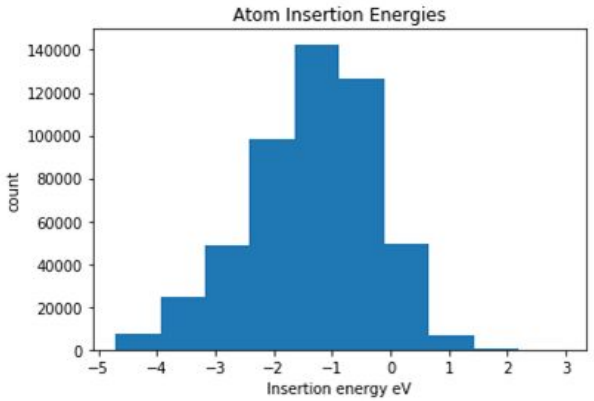
- ARE calculations for varied sizes



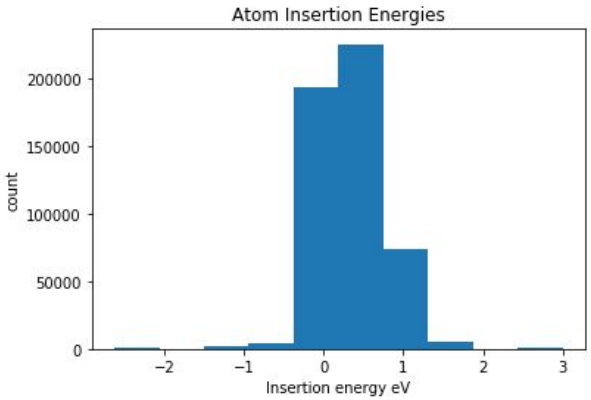



# Results

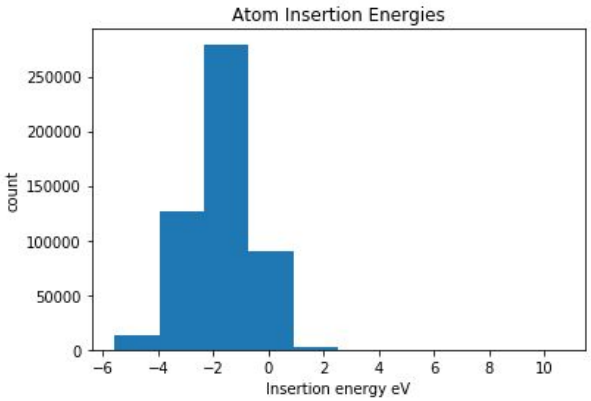
## Self Interstitial formation Energies




Amorphous silicon quenched at 10^-10 K/S




Crystal with one self interstitial




Amorphous silicon quenched at 10^-12 K/S

# Conclusion

- Found that Amorphous Silicon has negative vacancy formation energies.
- Results suggest negative vacancy formation energy is due to relaxation in structures.
- A prior experimental study shows bulk amorphous silicon continuously relaxing into a crystalline form [1].
- More research is required to fully understand this phenomenon.

1. S. Roorda, W. C. Sinke, J. M. Poate, D. C. Jacobson, S. Dierker, B. S. Dennis, D. J. Eaglesham, F. Spaepen, and P. Fuoss, Phys. Rev. B 44, 3702 (1991).

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