Computational methods for determining muon stopping sites: the case of crystalline silicon

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Problem: Where is the muon?

EXPERIMENTAL APPROACH

- Muonated Fe: follow the evolution of the muon frequency shift in a transverse field experiment as a function of the applied stress in a single Fe crystal[1]
- Muonated Si: stopping site of the BC muonium was determined using ALC results[2]

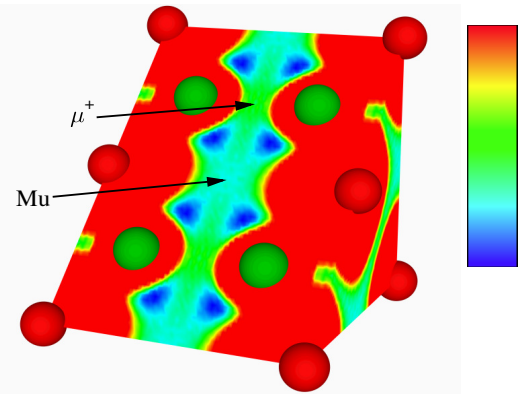
COMBINED THEORETICAL / EXPERIMENTAL APPROACH

- Muonated Fe_3O_4, ZnO and LiF: the theoretical calculations are used for testing different potential muon stopping sites

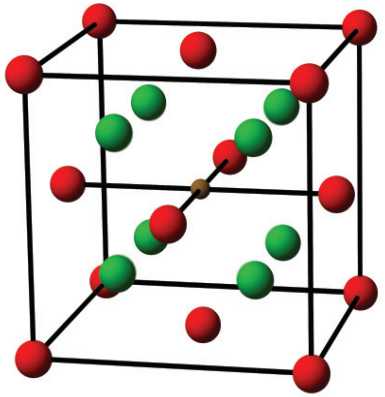
THEORETICAL APPROACH?

- Approach that relies on the analysis of the electrostatic potential of the bulk material obtained from Density Functional Theory (DFT) simulations. This is know as the **Unperturbed Electrostatic Potential Method (UEP)**

(b) CaF_2 (011)



Muonium in CaF_2

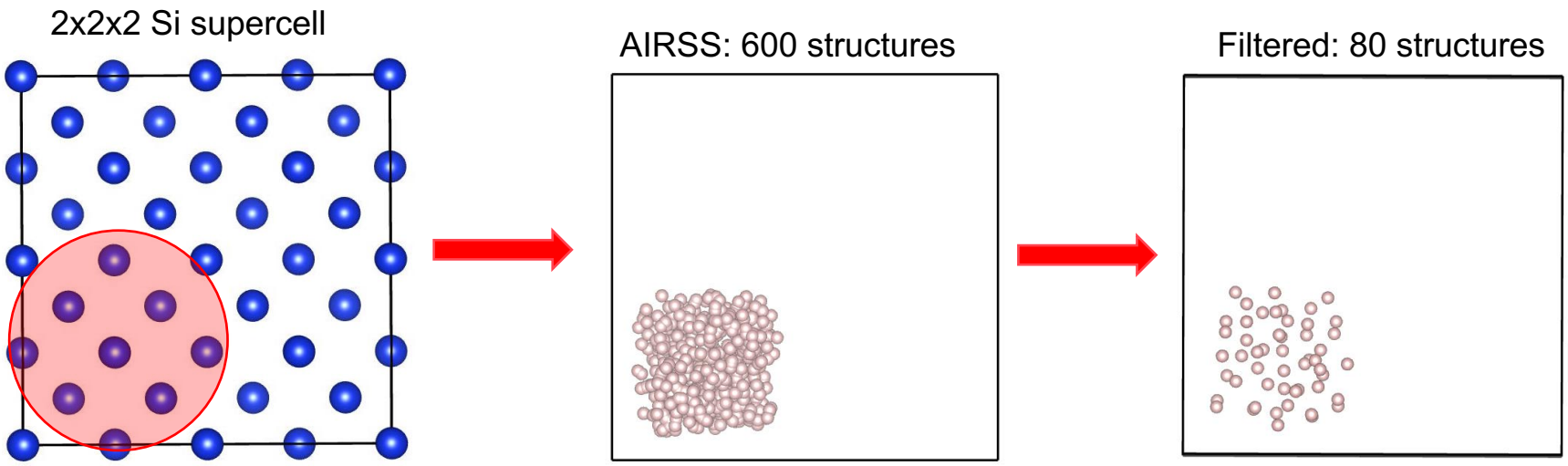


[1] W. J. Kossler, et. al., Phys. Rev. B **32**, 293, (1985)
[2] R. F. Kiefl, et. al., Phys. Rev. Lett. **60**, 224, (1988)
J. Moller, *et al.,* Phys. Rev. B **87**, 121108(R) (2013)

AIRSS methodology in crystalline Si

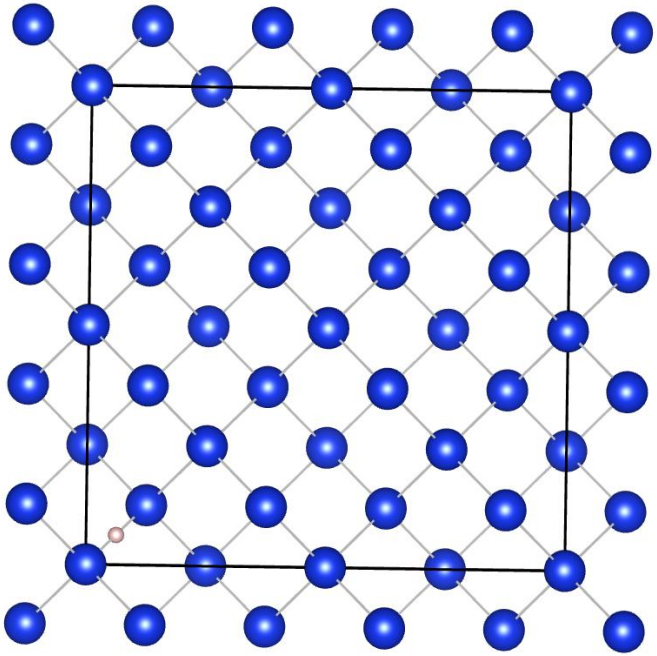
Ab Initio Random Structure Searching (AIRSS)

1) Build 2x2x2 Si supercell
2) Define spherical region to randomly locate muonium atoms
3) Generate muonated structures placing muonium in randomised positions within the chosen region
4) Filter generated structures to remove redundant structures
5) Relax filtered structures using calculated DFT forces



A. J. Morris, *et. al.,* Phys. Rev. B **80**, 144112 (2009).
C. Pickard et. al. J. Phys.: Condens. Matter **23** (2011) 053201

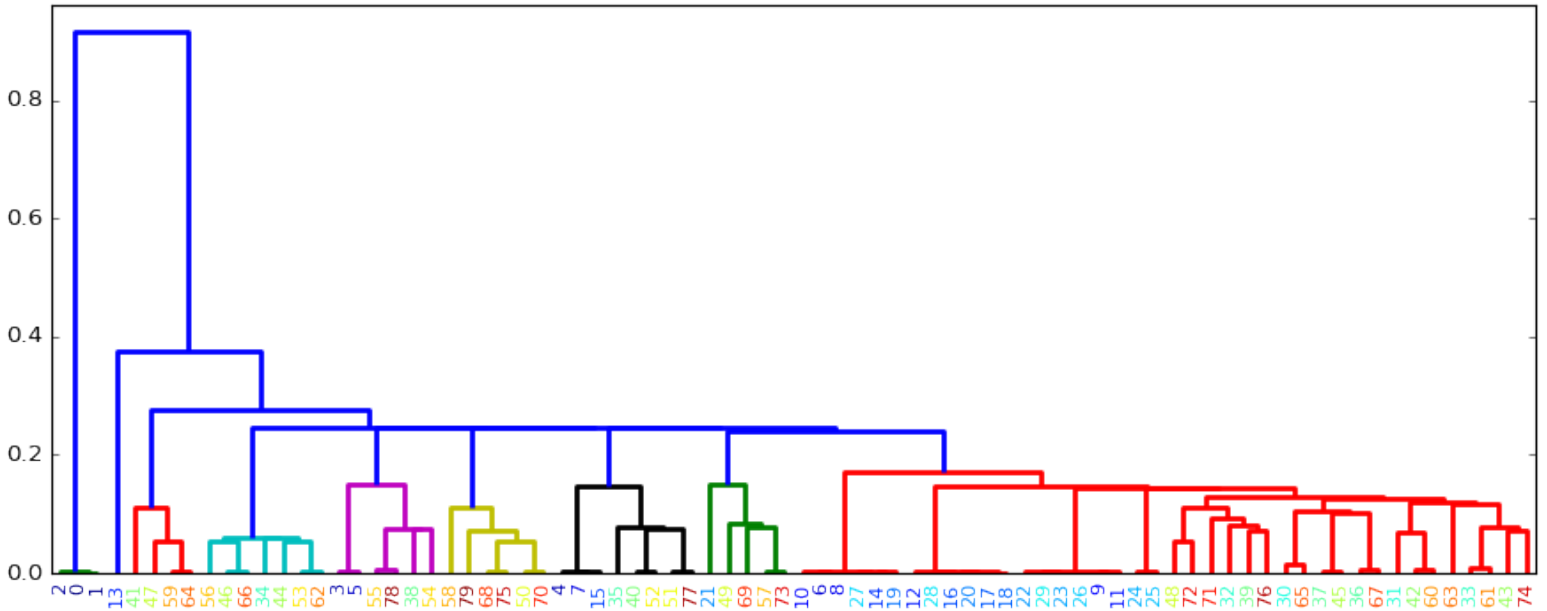
Technical details of calculations



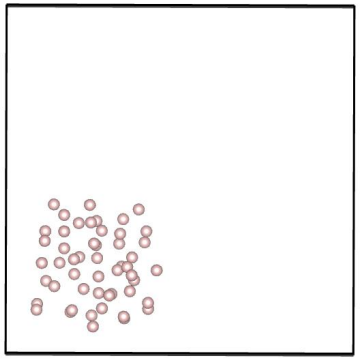
UK National Supercomputing Service

- High-throughput DFT calculations performed with the CASTEP code, using norm-conserving pseudopotentials.
- Calculations have been done for neutral muonium in crystalline 2x2x2 Silicon supercells.
- GGA (PBE) treatment of the exchange and correlation.
- Spin polarized calculation with initial spin in muonium.
- Generated 600 structures with AIRSS, which were then filtered to 80.
- Cluster analysis performed on the resulting 80 structures.

Cluster Analysis: hierarchical



Filtered: 80 structures

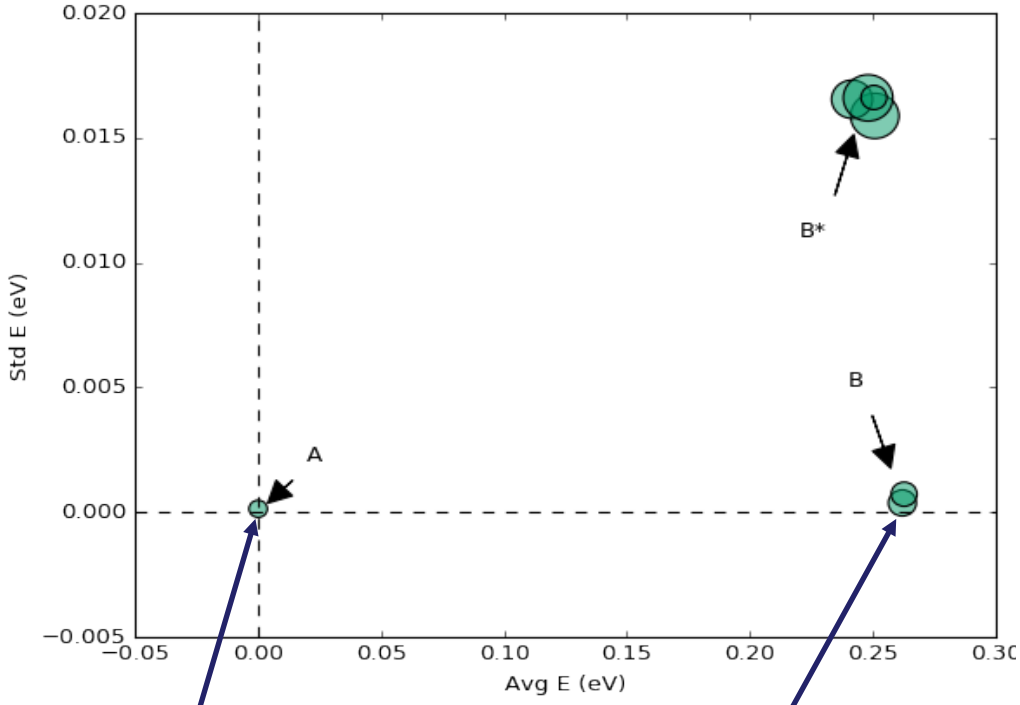


- Define 4D vector: (E_T, mu_x, mu_y, mu_z)
- Look for “closeness” in 4D space
- 7 clusters identified

Python library Soprano (CCP NC) https://ccpforge.cse.rl.ac.uk/gf/project/soprano/

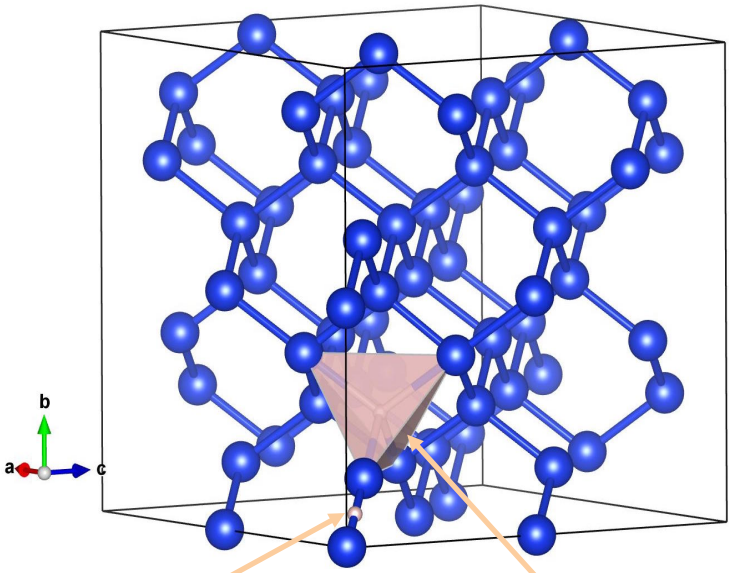
SOPRANO

Cluster Analysis: k-means



Cluster representing
Mu_BC stopping site

Cluster representing
Mu_T stopping ‘region’



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SOPRANO

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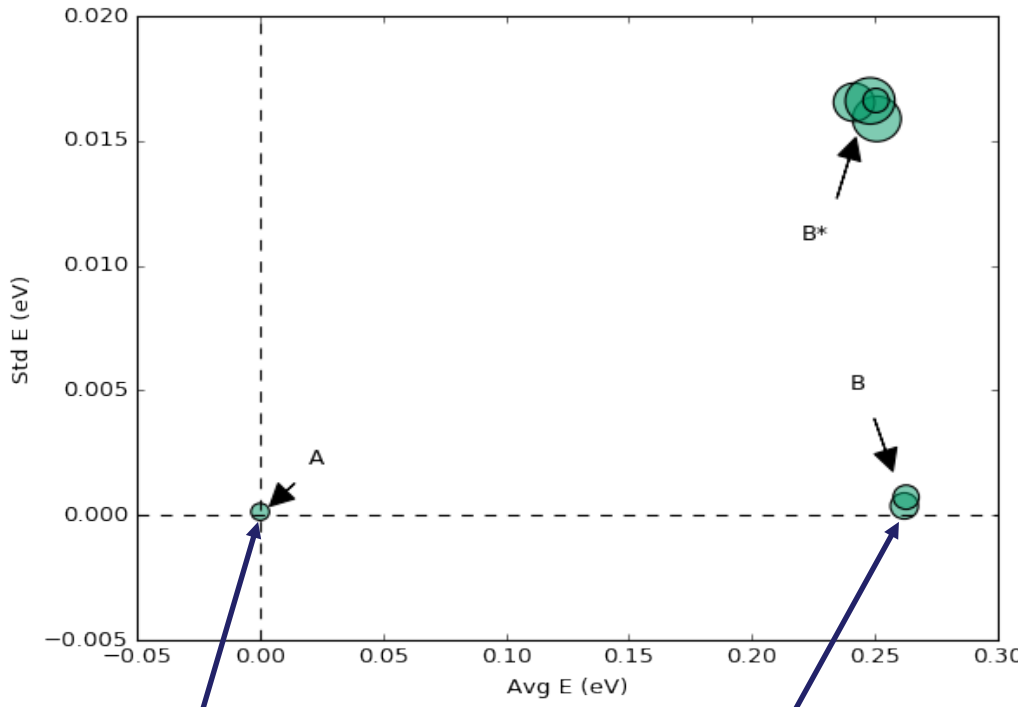

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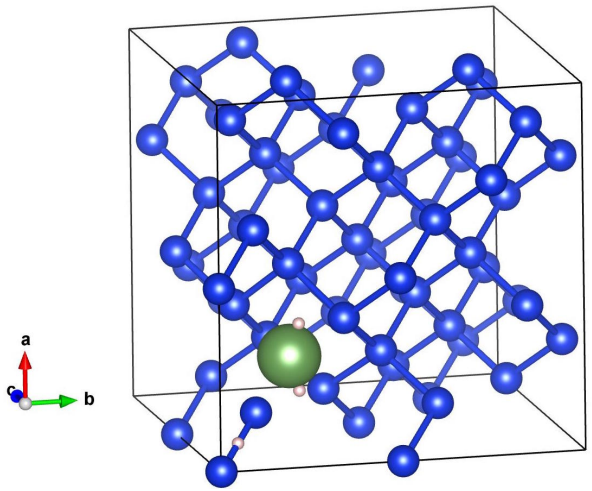

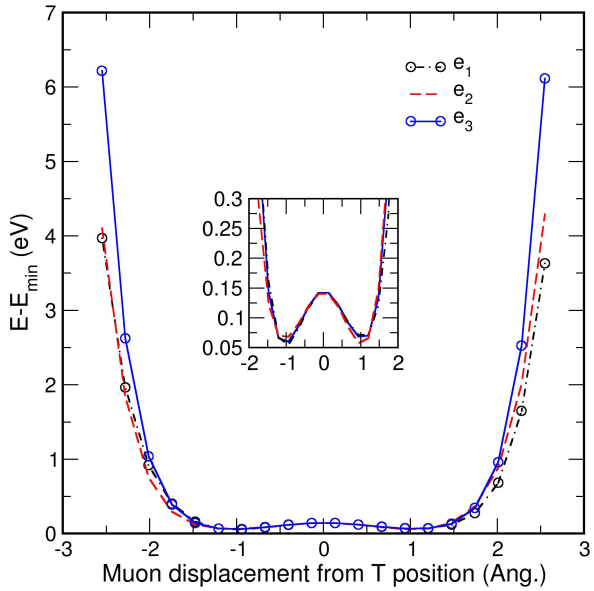

B. Patterson., Rev. Mod. Phys. **60**, 69, (1988)

Conclusions

- We are developing a computational method to **estimate the stopping sites of muons** in crystalline materials
- Our method **complements** the known methodologies used for predicting the muon stopping sites.
- The method utilizes **DFT calculations** combined with the **AIRSS methodology** for generating a set of potential muonated structures
- **Machine learning techniques** are then used to efficiently search for clusters in these structures
- The **Python library Soprano** is used to implement the method and identify theclusters
- The method **predicted** the stopping site for **BC muonium** in Si and the stopping 'region' for muoniums in the **tetragonal** region in Si
- We will be testing the method in Diamond, Germanium, LiF, NaF and NiO and MnO.