

## Crystal Structure:

Ge (Diamond FCC)

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CIF Source:

Cooper A S

Acta Crystallographica 15 (1962) 578-582

Precise lattice constants of germanium, aluminum, gallium arsenide, uranium, sulphur, quartz and sapphire

Locality: synthetic

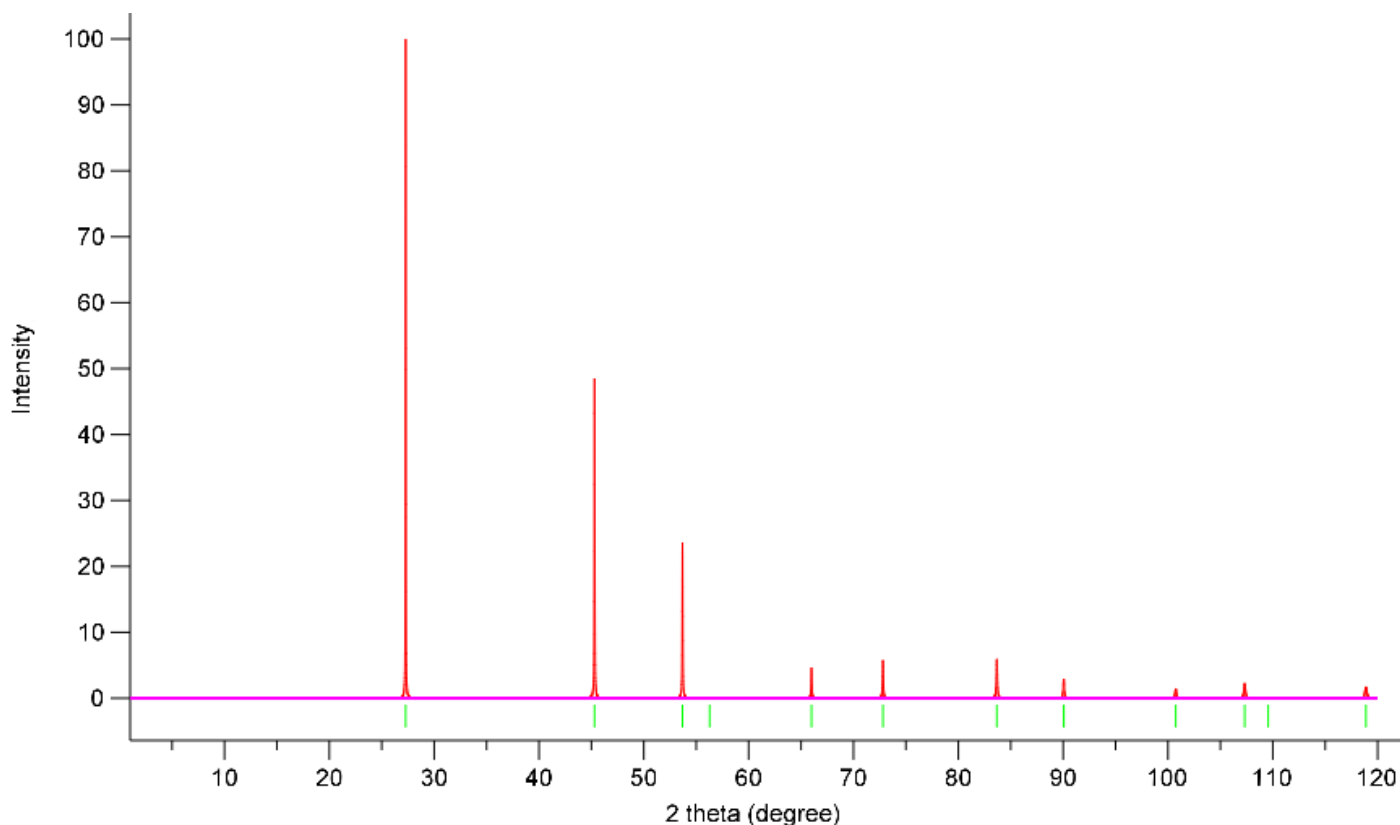
Sample: at T = 24.6 C

\_database\_code\_amcsd 0009269

<http://rruff.geo.arizona.edu/AMS/download.php?id=10526.cif&down=cif>

## Simulated Powder XRD using VESTA:

X-Ray Wavelength: 1.54059 Angstrom



## Simulation 1: GGA

Pseudopotential Used:

Ge.pbe-n-rrkjus\_psl.1.0.0.UPF

PP Type: Ultrasoft

Exchange Correlation Functional: PBE-GGA

Non-linear core corrections are used.

Wavefunction Energy Cutoff: 20 Ry  
Charge Density Energy Cutoff: 220 Ry  
k - mesh: 8x8x8  
Run Type: GGA-PBE

Total Energy vs Cutoff:

Cutoff(Ry)	Total Energy(Ry)
5	-93.78629932
10	-94.20616615
15	-94.25531942
18	-94.26356054
20	-94.26832366
22	-94.27156940
25	-94.27517056

## Optimized Coordinates and Lattice Parameters:

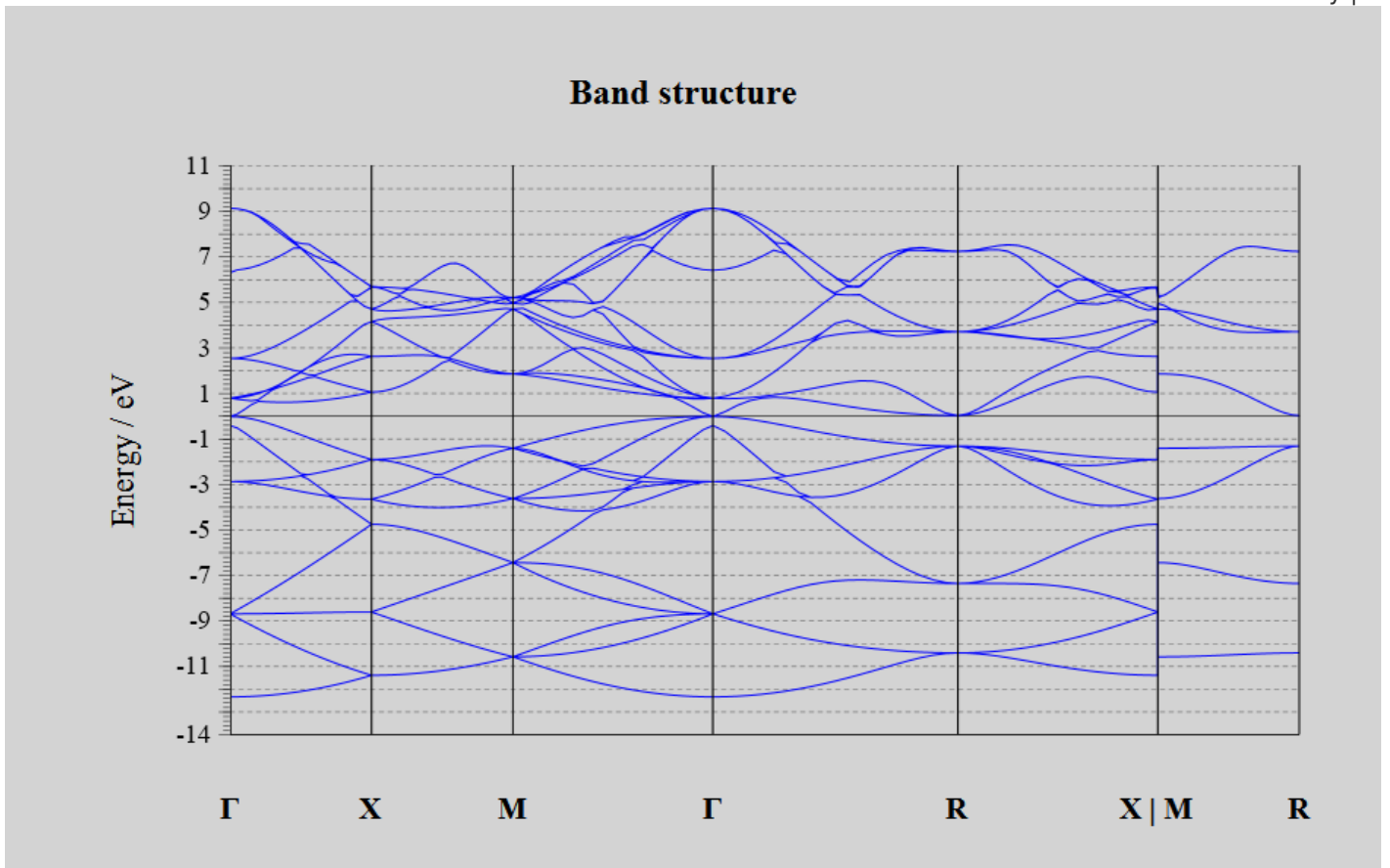
CELL\_PARAMETERS {angstrom}

5.766148	0.000000	0.000000
0.000000	5.766148	0.000000
0.000000	0.000000	5.766148

ATOMIC\_POSITIONS {angstrom}

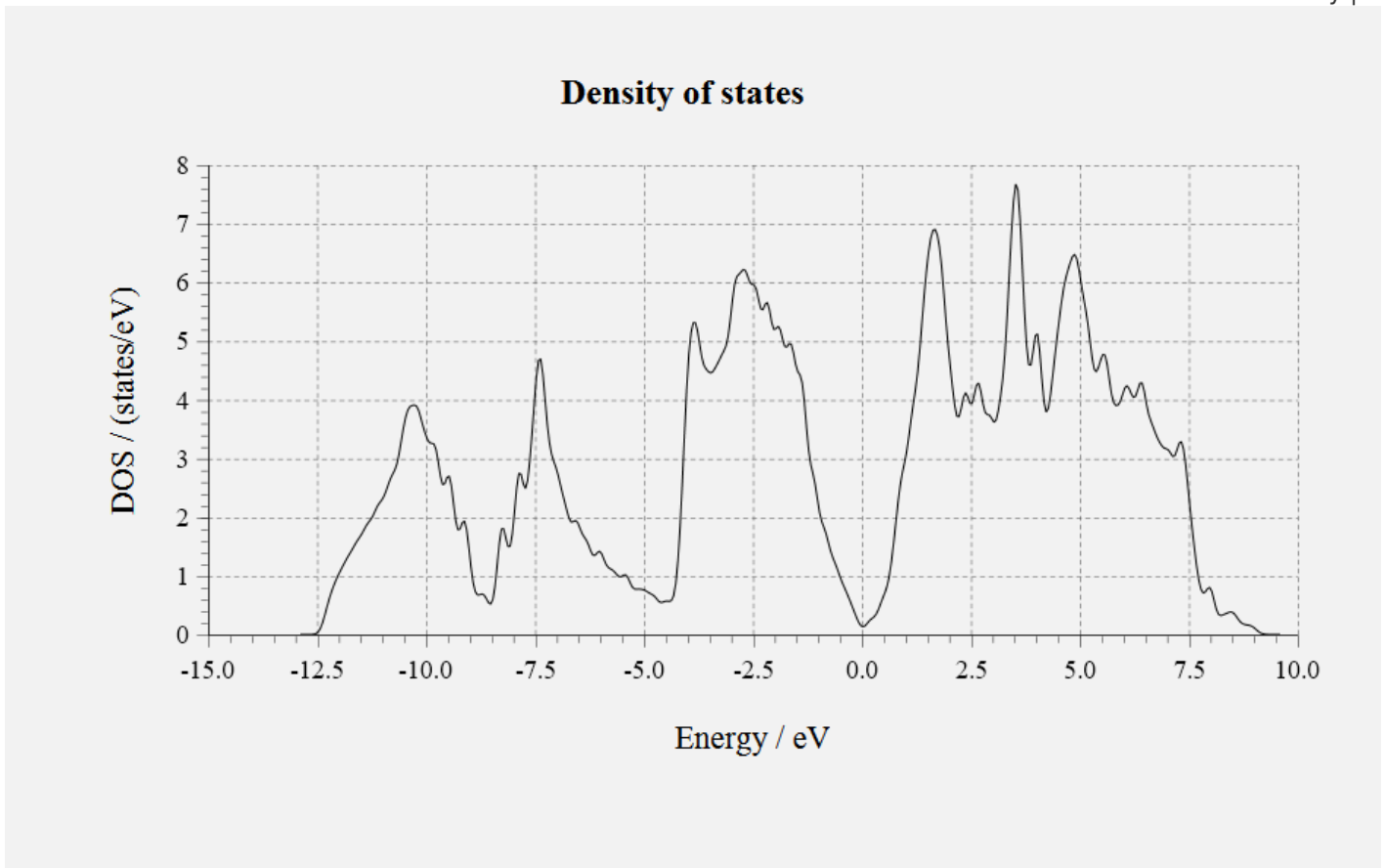
Ge	0.000000	0.000000	0.000000
Ge	0.000000	2.883074	2.883074
Ge	2.883074	0.000000	2.883074
Ge	2.883074	2.883074	0.000000
Ge	4.324611	4.324611	1.441537
Ge	4.324611	1.441537	4.324611
Ge	1.441537	4.324611	4.324611
Ge	1.441537	1.441537	1.441537

## Bandstructure:



Band-gap: 0 eV

Density of States(DOS):



## Input Files:

[Ge DFCC Input files for Quantum Espresso](#)

## Acknowledgements:

I acknowledge the use of the following tools and packages in order to produce the above simulations.

Quantum Espresso(for DFT based simulations): <http://www.quantum-espresso.org/>

BURAI(for visualization and as a GUI for QE): <http://nisihara.wixsite.com/burai>

VESTA(for visualization and XRD simulations): <http://jp-minerals.org/vesta/en/>

## References and Resources

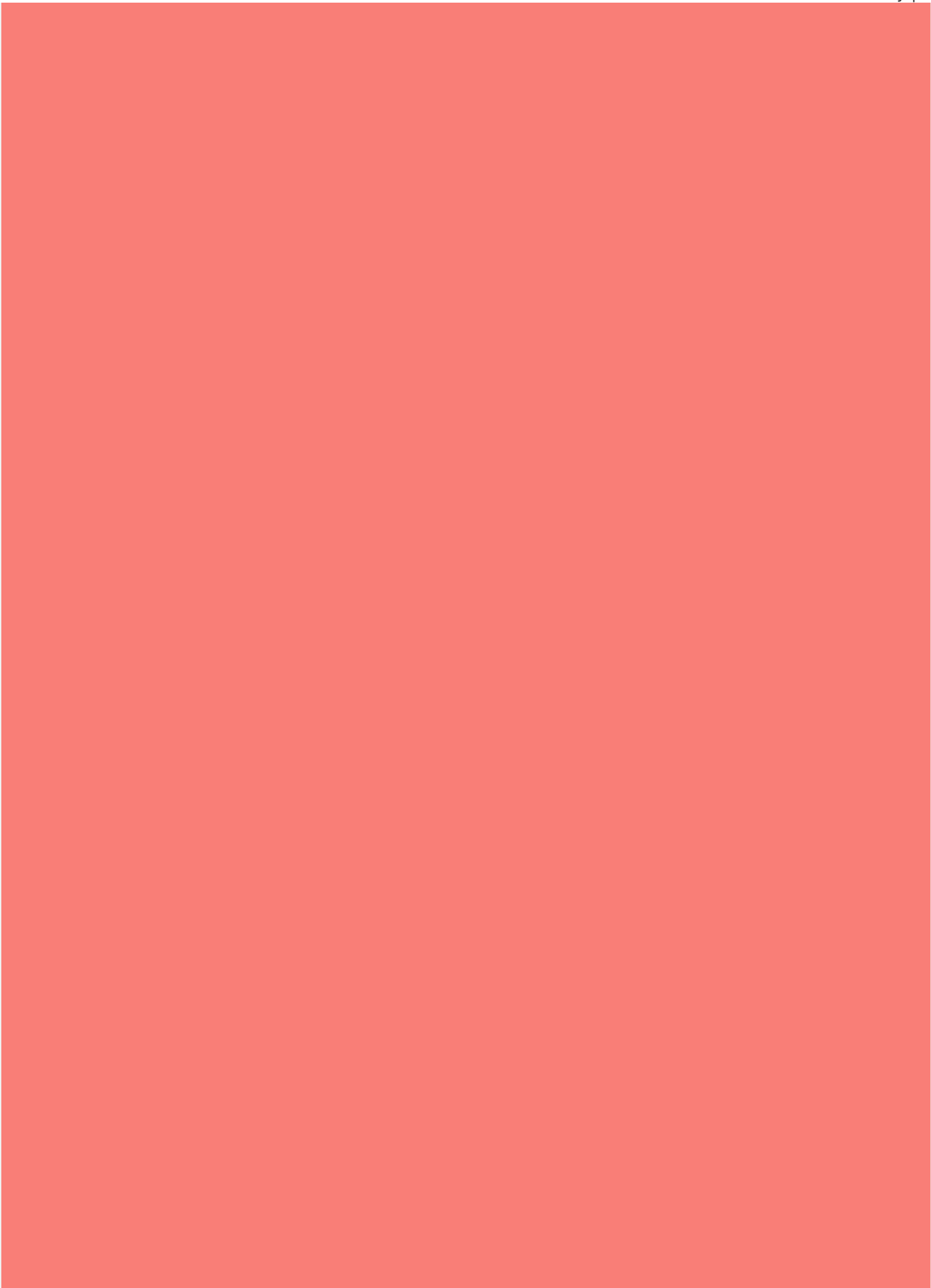


### Manas Sharma

I'm a physicist specializing in computational material science with a PhD in Physics from Friedrich-

Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, and Machine Learning related apps and software from time to time. Can code in most of the popular languages. I like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

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