Crystal Structure:

ZnS (Wurtzite)

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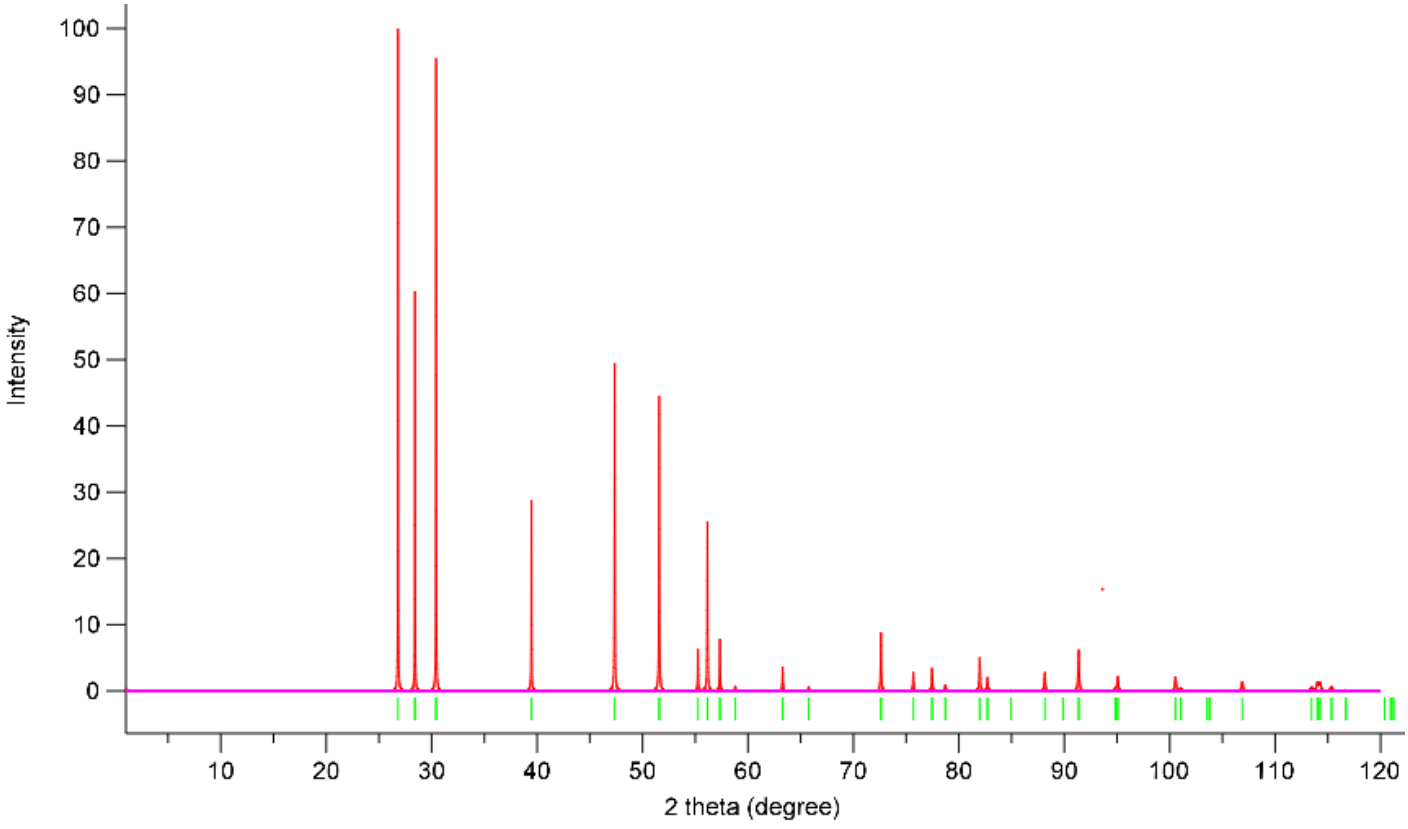
CIF Source:
Ulrich F, Zachariasen W H
Zeitschrift fur Kristallographie 62 (1925) 260-273
Ueber die kristallstruktur des alpha- und beta-CdS, sowie des wurtzits
Locality: synthetic
_database_code_amcsd 0010493
http://rruff.geo.arizona.edu/AMS/download.php?id=12087.cif&down=cif

Simulated Powder XRD using VESTA:

X-Ray Wavelength: 1.54059 Angstrom



Powder XRD pattern simulation of ZnS (wurtzite)

Simulation 1: GGA

Pseudopotential Used:
Zn.pbe-dn-rrkjus_psl.1.0.0.UPF
S.pbe-nl-rrkjus_psl.1.0.0.UPF

PP Type: Ultrasoft
Exchange Correlation Functional: PBE-GGA
Non-linear core corrections are used.

Wavefunction Energy Cutoff: 43 Ry
Charge Density Energy Cutoff: 473 Ry
k – mesh: 8x8x8
Run Type: GGA-PBE

Total Energy vs Cutoff:

Cutoff(Ry)	Total Energy(Ry)
25	-337.89838640
30	-338.63846151
35	-338.77517997
40	-338.78951530
43	-338.78996329
45	-338.79066397

Optimized Coordinates and Lattice Parameters:

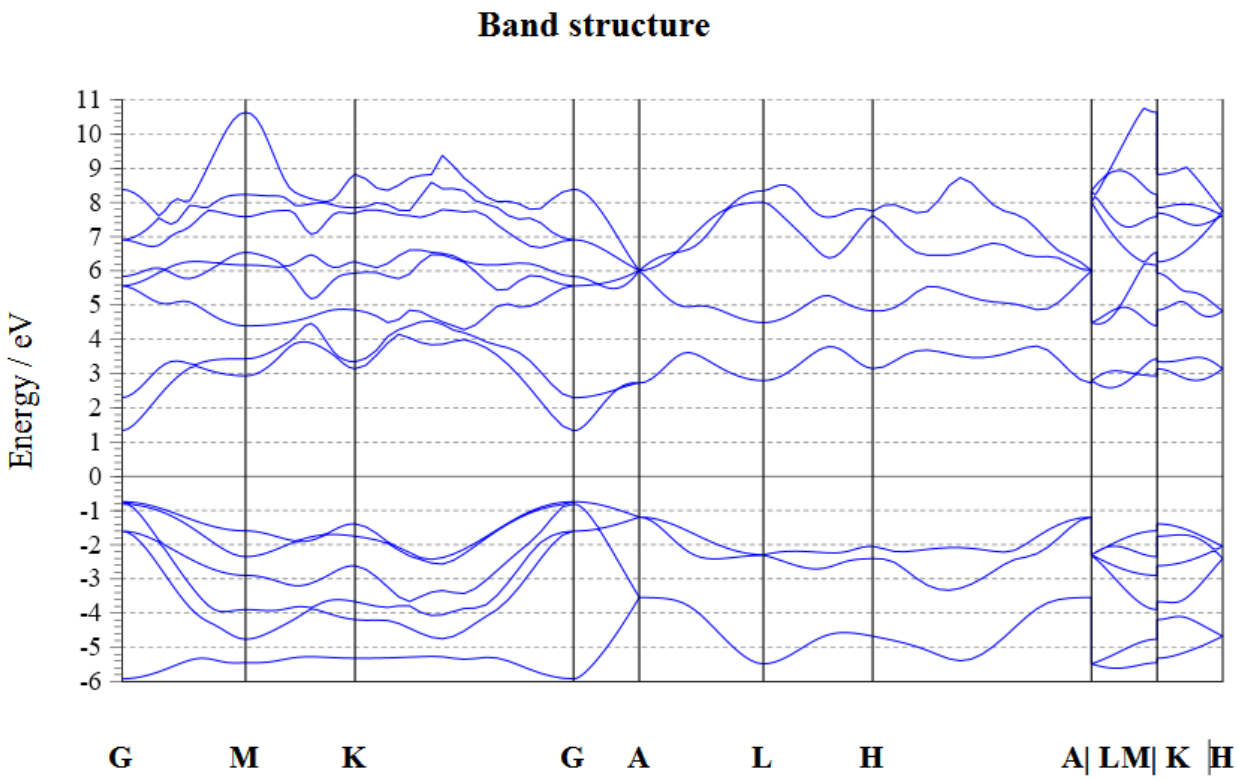
CELL_PARAMETERS {angstrom}

3.844996	0.000007	0.000000
-1.922492	3.329854	-0.000001
0.000001	-0.000001	6.299811

ATOMIC_POSITIONS {angstrom}

Zn	-0.000009	2.219920	0.000630
Zn	1.922494	1.109974	3.150536
S	-0.000007	2.219920	2.361798
S	1.922493	1.109972	5.511704

Bandstructure:

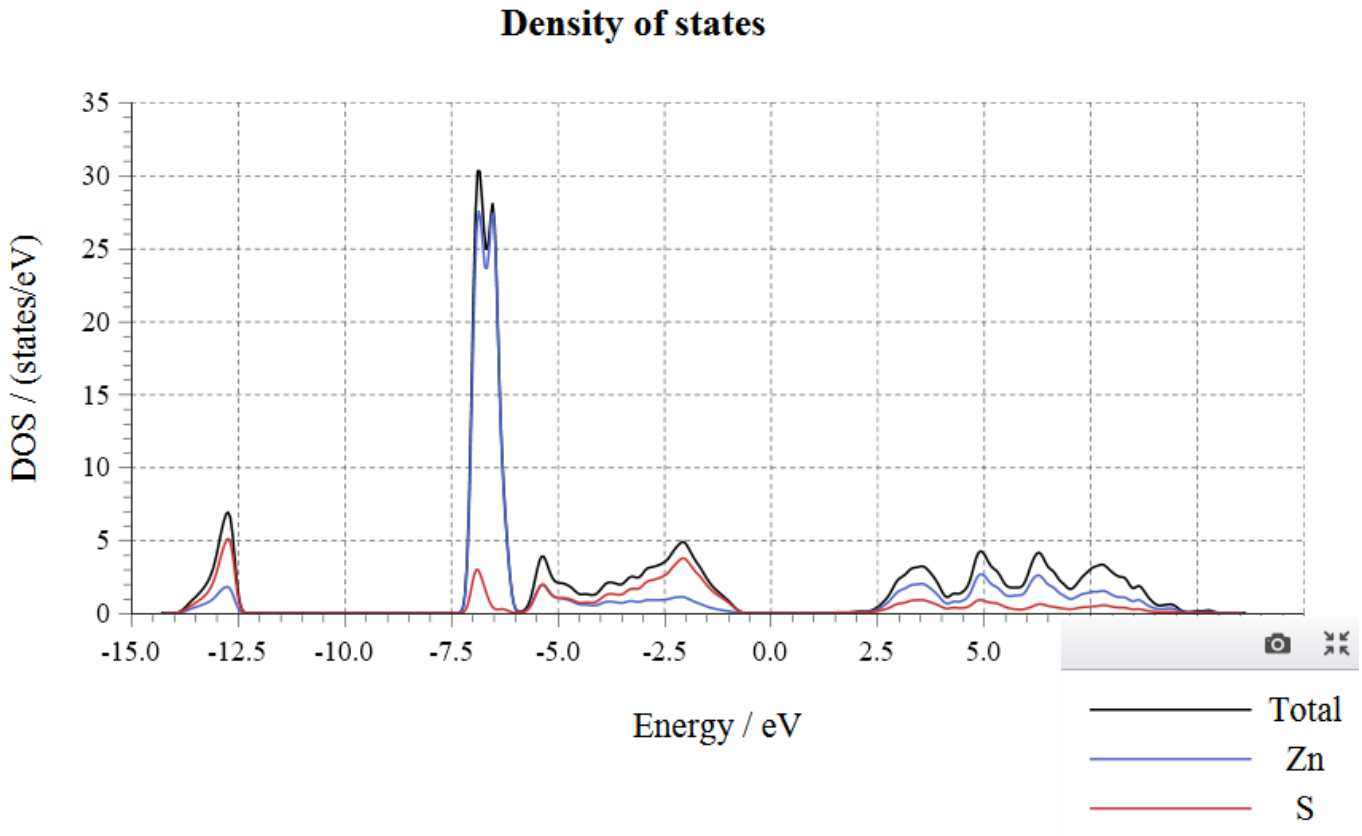


Bandstructure of ZnS (wurtzite) along high symmetry points

highest occupied, lowest unoccupied level (ev): 5.5547 7.6264

Band-gap: 2.0717 eV

Density of States(DOS):



Density of states of ZnS (wurtzite)

Input Files:

Input files ZnS wurtzite 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

https://arxiv.org/pdf/1312.4272.pdf

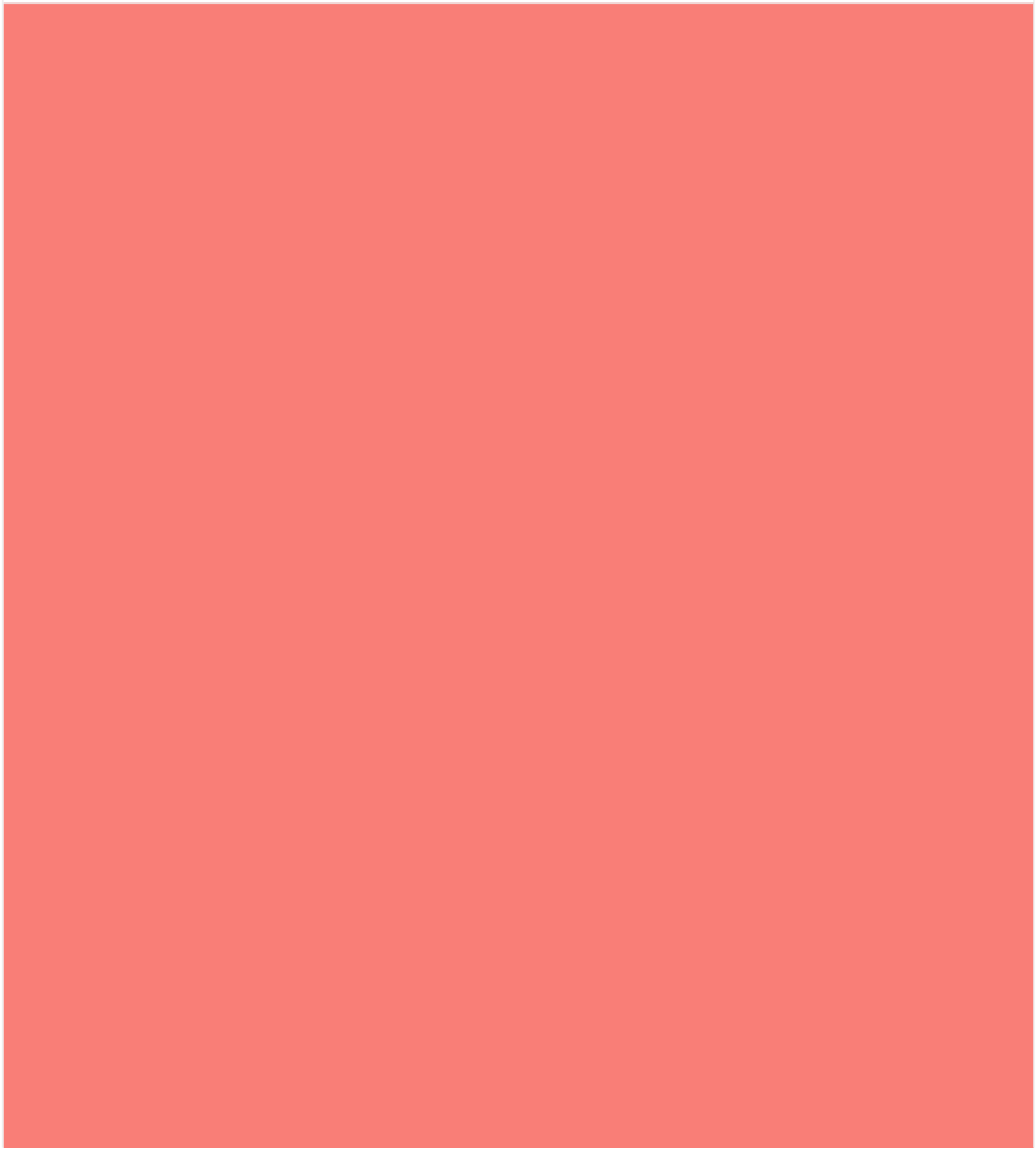
http://pubs.rsc.org/en/content/articlelanding/2014/ra/c4ra05960c/unauth

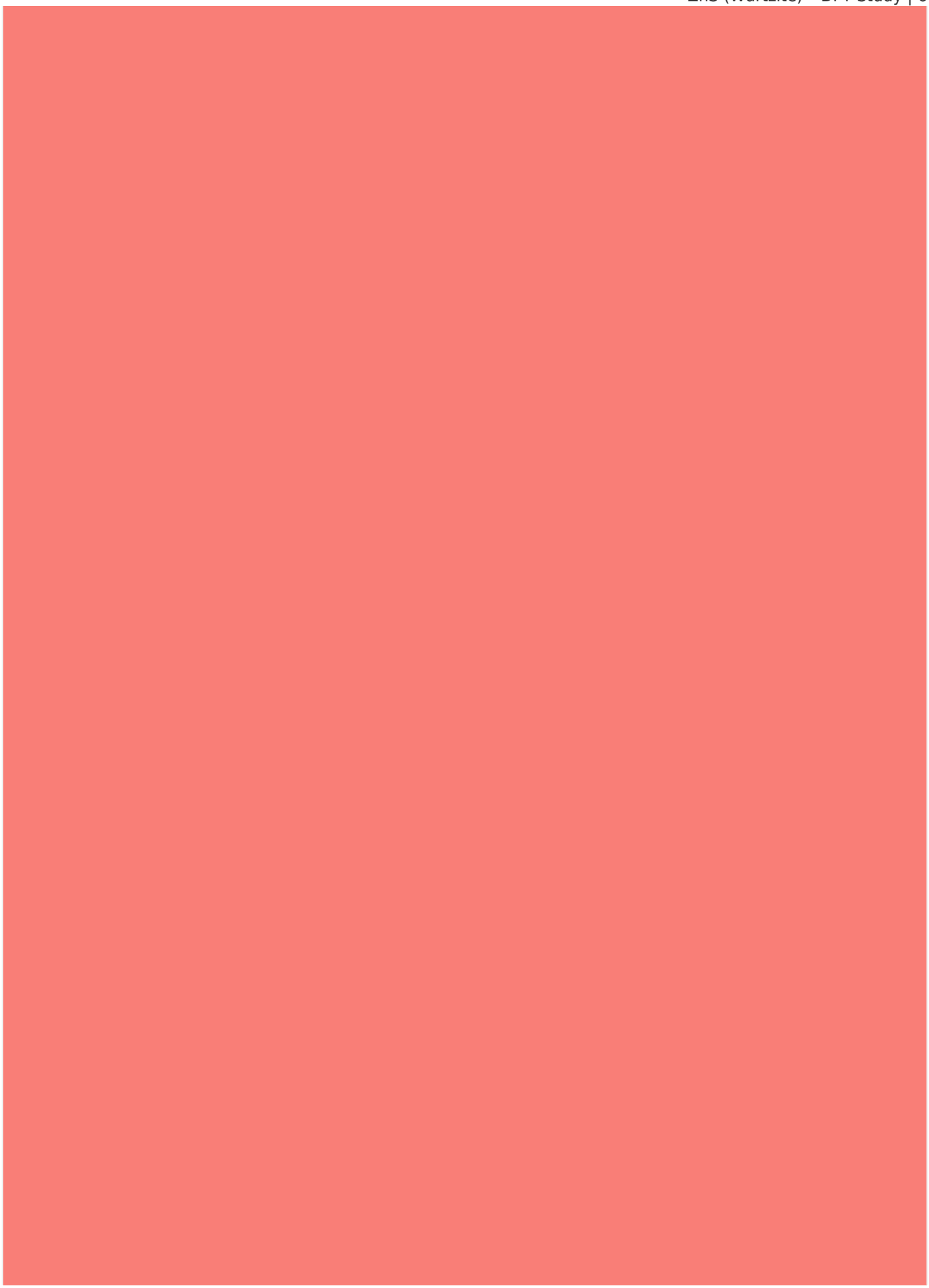
http://pubs.rsc.org/en/content/articlelanding/2015/cp/c5cp04623h/unauth#!divAbstract

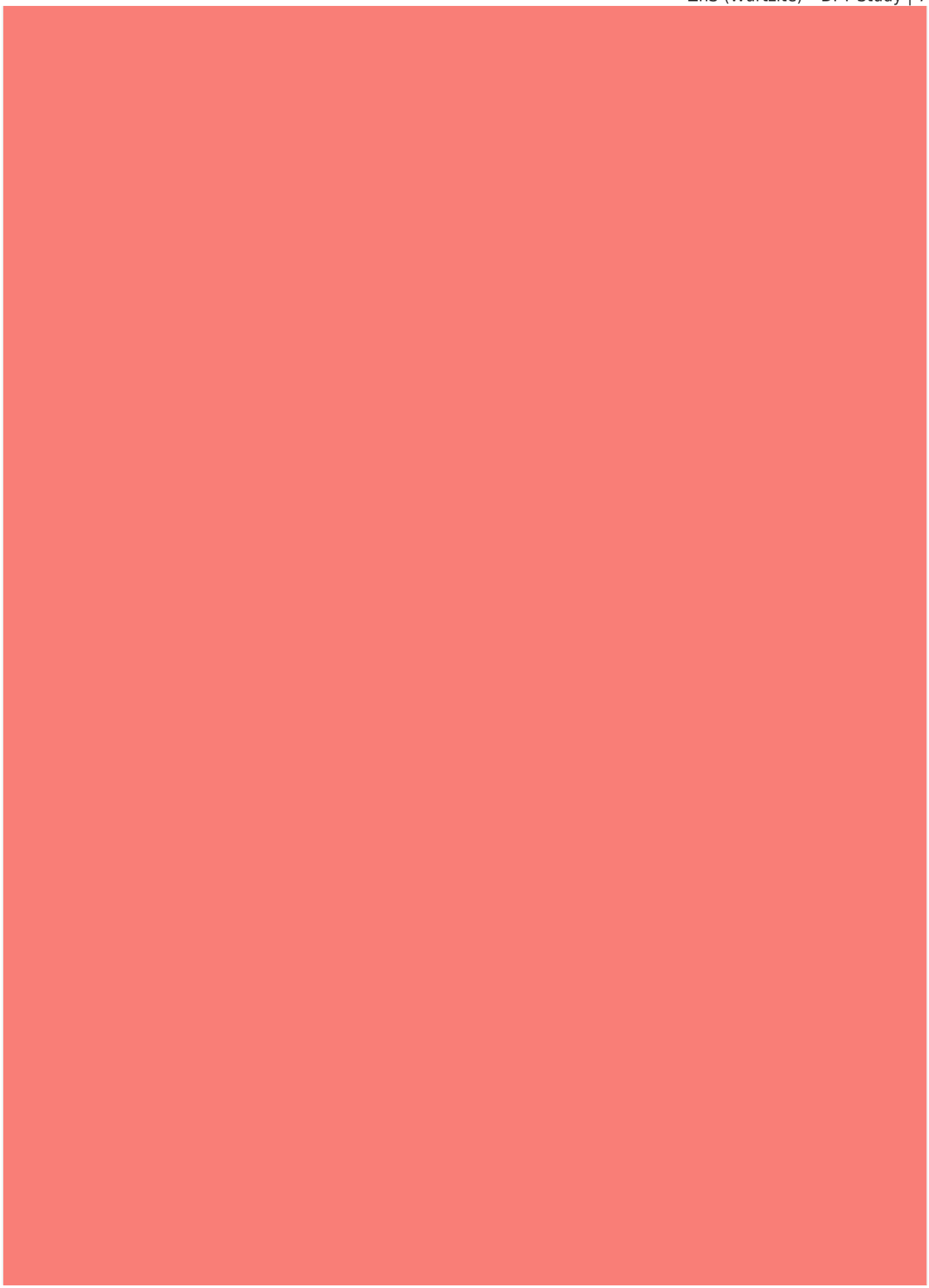
Manas Sharma

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.

manas.bragitoff.com/







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