Crystal Structure:

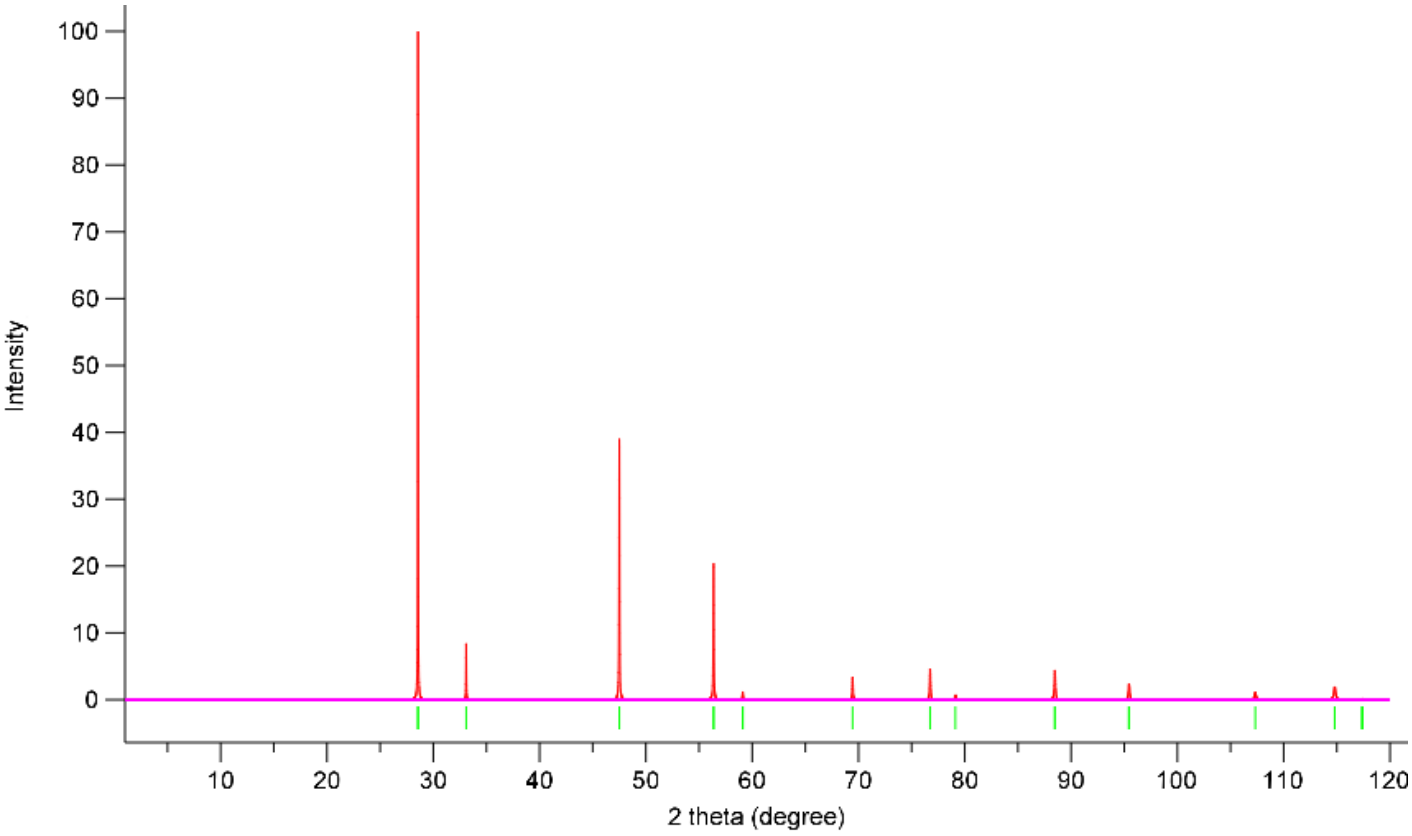
ZnS (Cubic)

About/Help

CIF Source:
American Mineralogist 46 (1961) 1399-1411
Unit-cell edges of natural and synthetic sphalerites
Locality: synthetic
_database_code_amcsd 0000110
http://rruff.geo.arizona.edu/AMS/download.php?id=00200.cif&down=cif

Simulated Powder XRD using VESTA:

X-Ray Wavelength: 1.54059 Angstrom



XRD Pattern simulation of ZnS (cubic) using VESTA

Simulation 1: GGA

Pseudopotential Used:

Zn.pbe-dn-rrkjus_psl.1.0.0.UPF
S.pbe-nl-rrkjus_psl.1.0.0.UPF

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	-675.79600658
30	-677.27787004
35	-677.55108596
40	-677.58002140
43	-677.58093776
45	-677.58235107
46	-677.58348336
47	-677.58488913

Optimized Coordinates and Lattice Parameters:

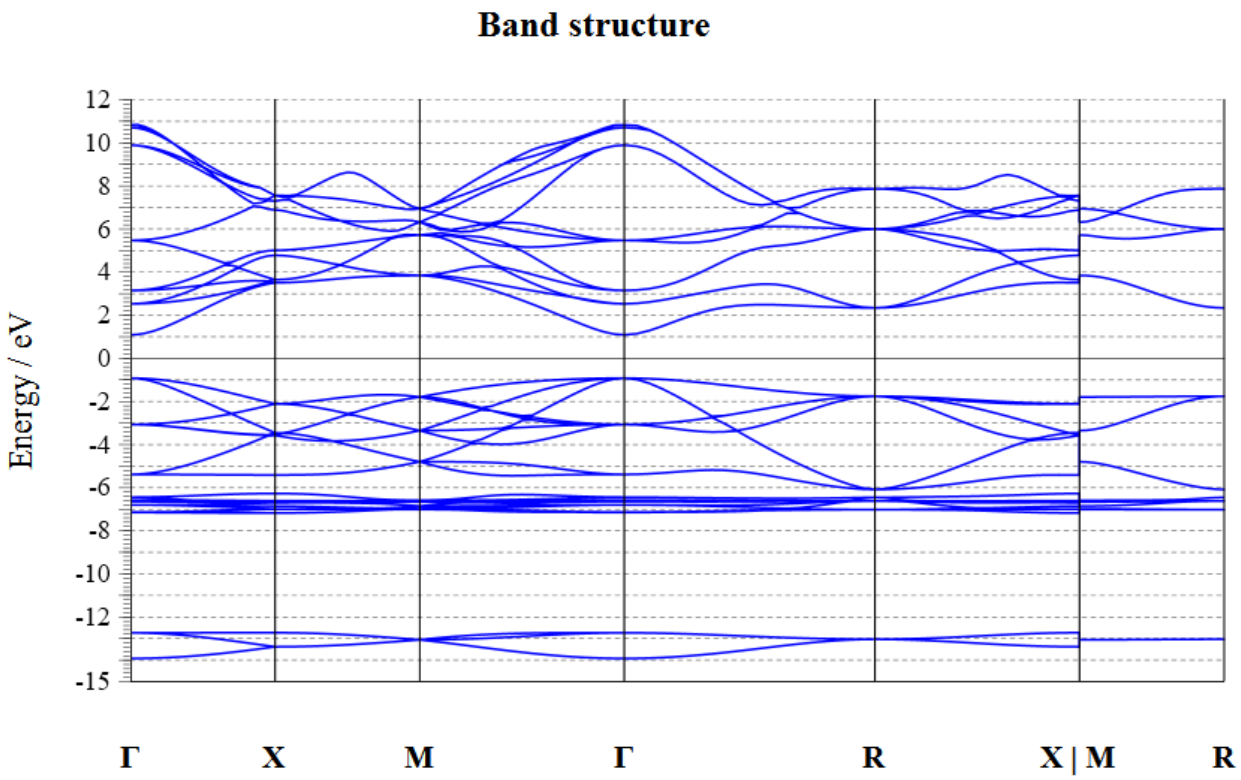
CELL_PARAMETERS {angstrom}

5.441778	0.000000	0.000000
0.000000	5.441778	0.000000
0.000000	0.000000	5.441778

ATOMIC_POSITIONS {angstrom}

Zn	0.000000	0.000000	0.000000
Zn	0.000000	2.720889	2.720889
Zn	2.720889	0.000000	2.720889
Zn	2.720889	2.720889	0.000000
S	1.360446	1.360446	1.360446
S	1.360446	4.081332	4.081332
S	4.081332	1.360446	4.081332
S	4.081332	4.081332	1.360446

Bandstructure:

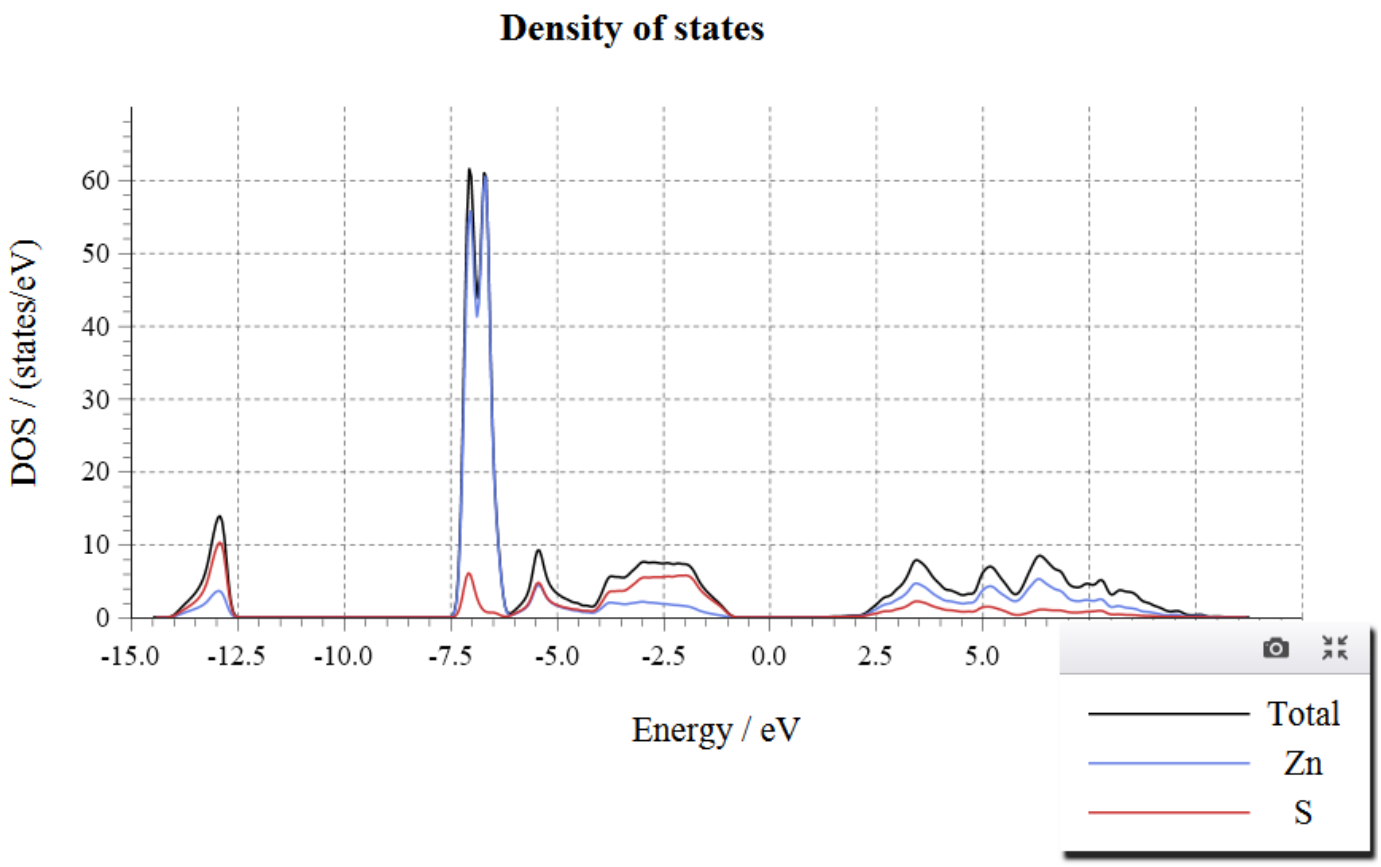


Bandstrucutre of ZnS (cubic) along high symmetry points

highest occupied, lowest unoccupied level (ev): 5.5514 7.5571

Band Gap= 2.006 eV

Density of States(DOS):



Density of states ZnS (cubic)

Input Files:

Input Files ZnS Cubic 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/

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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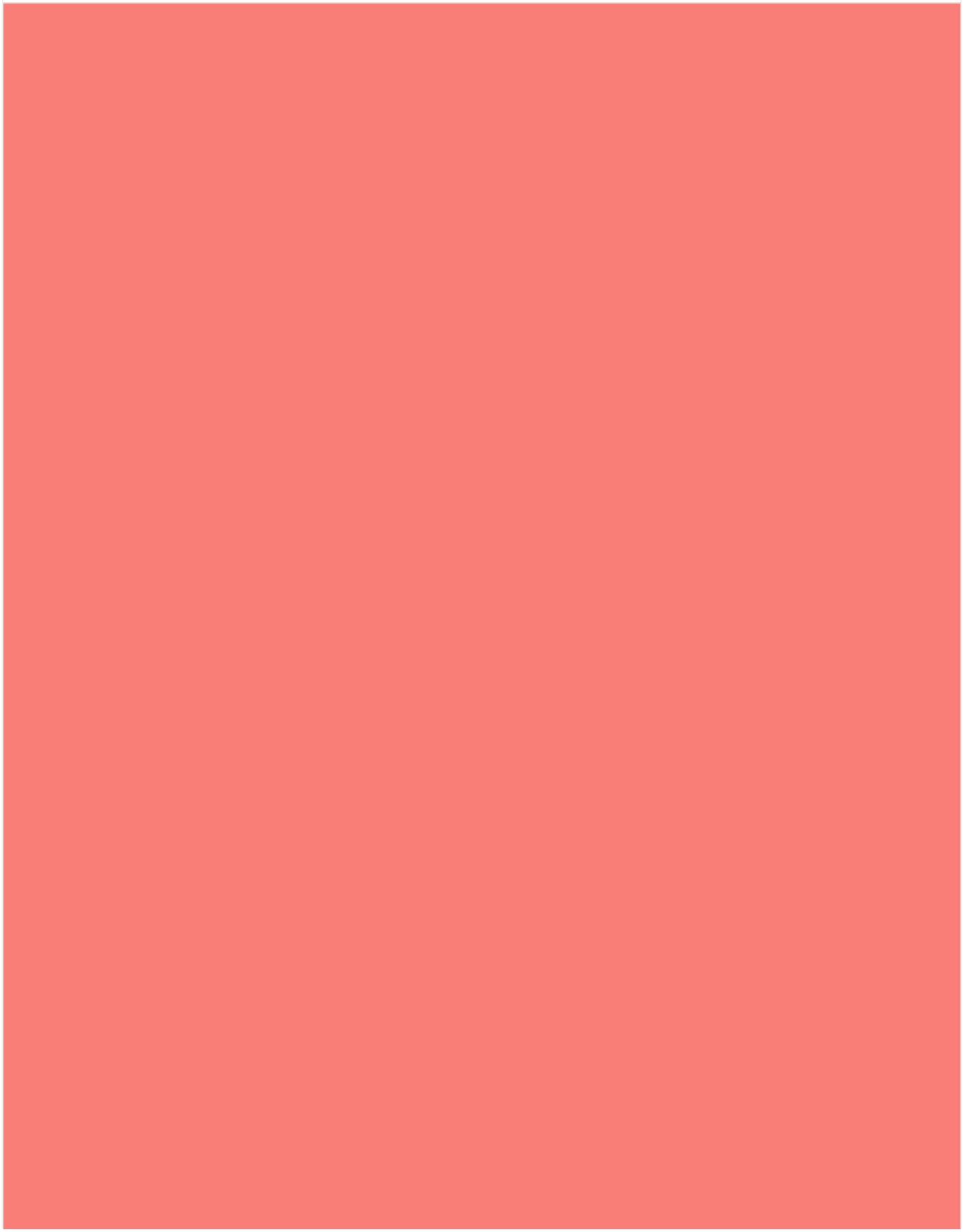

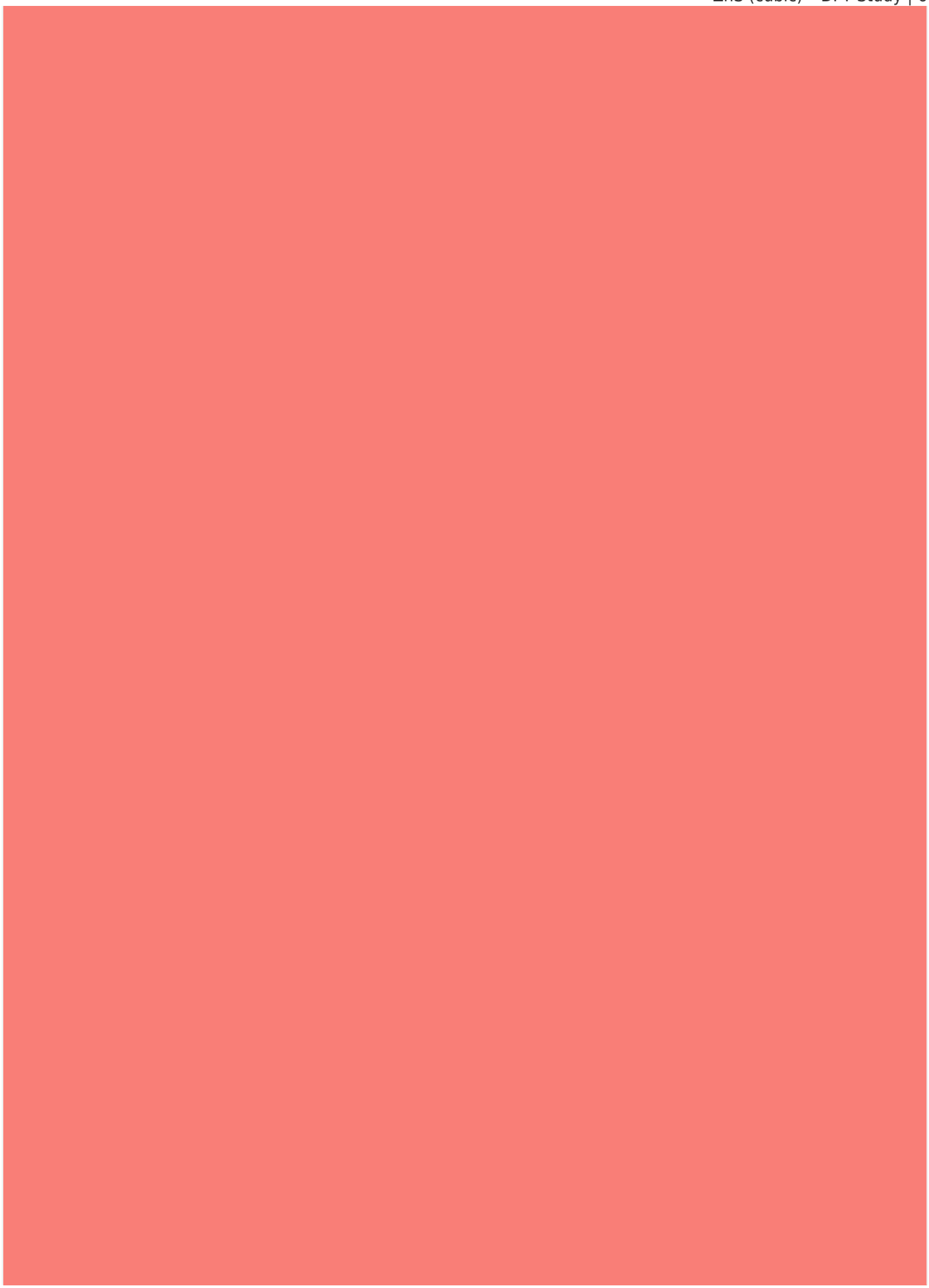

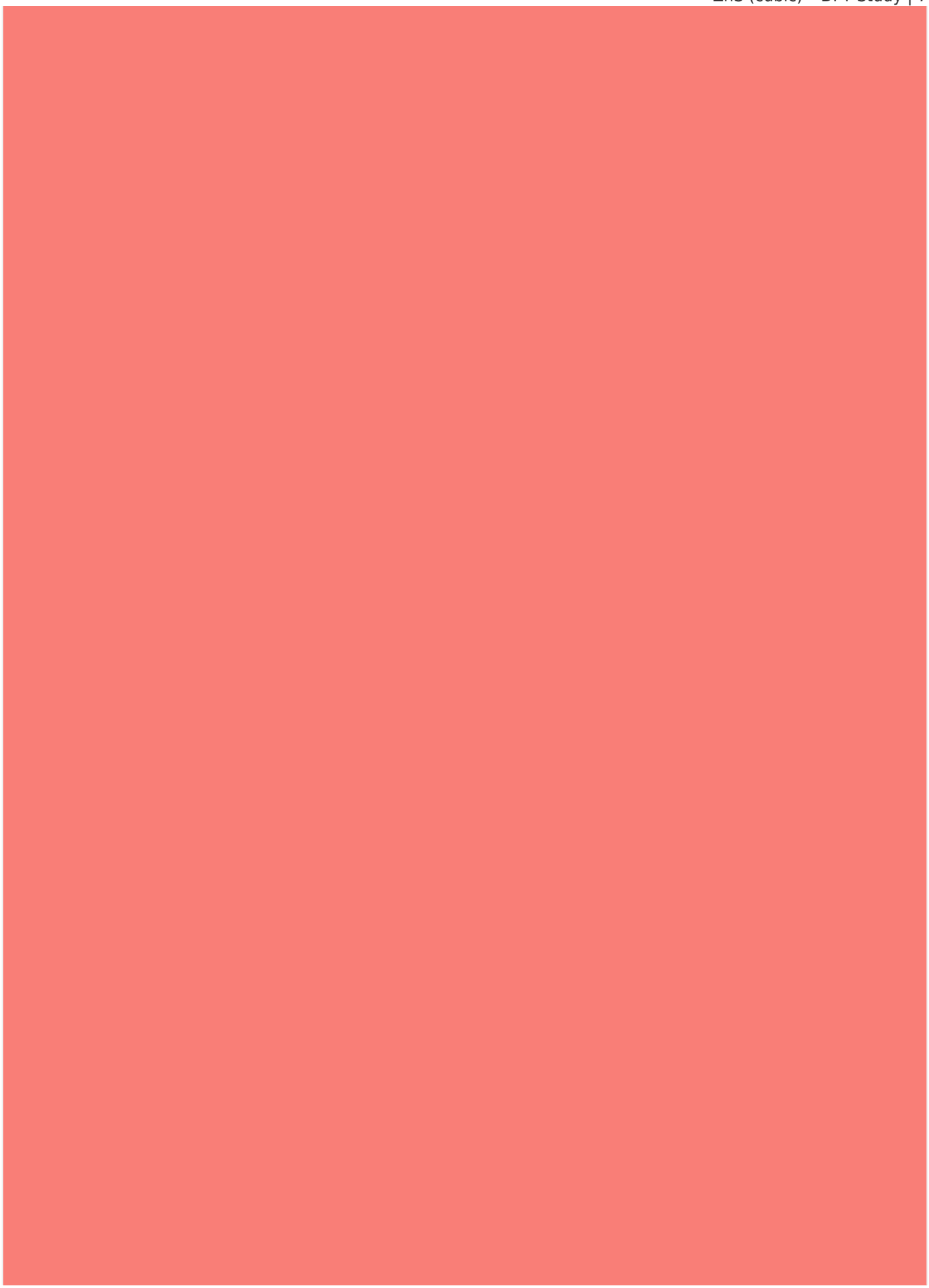

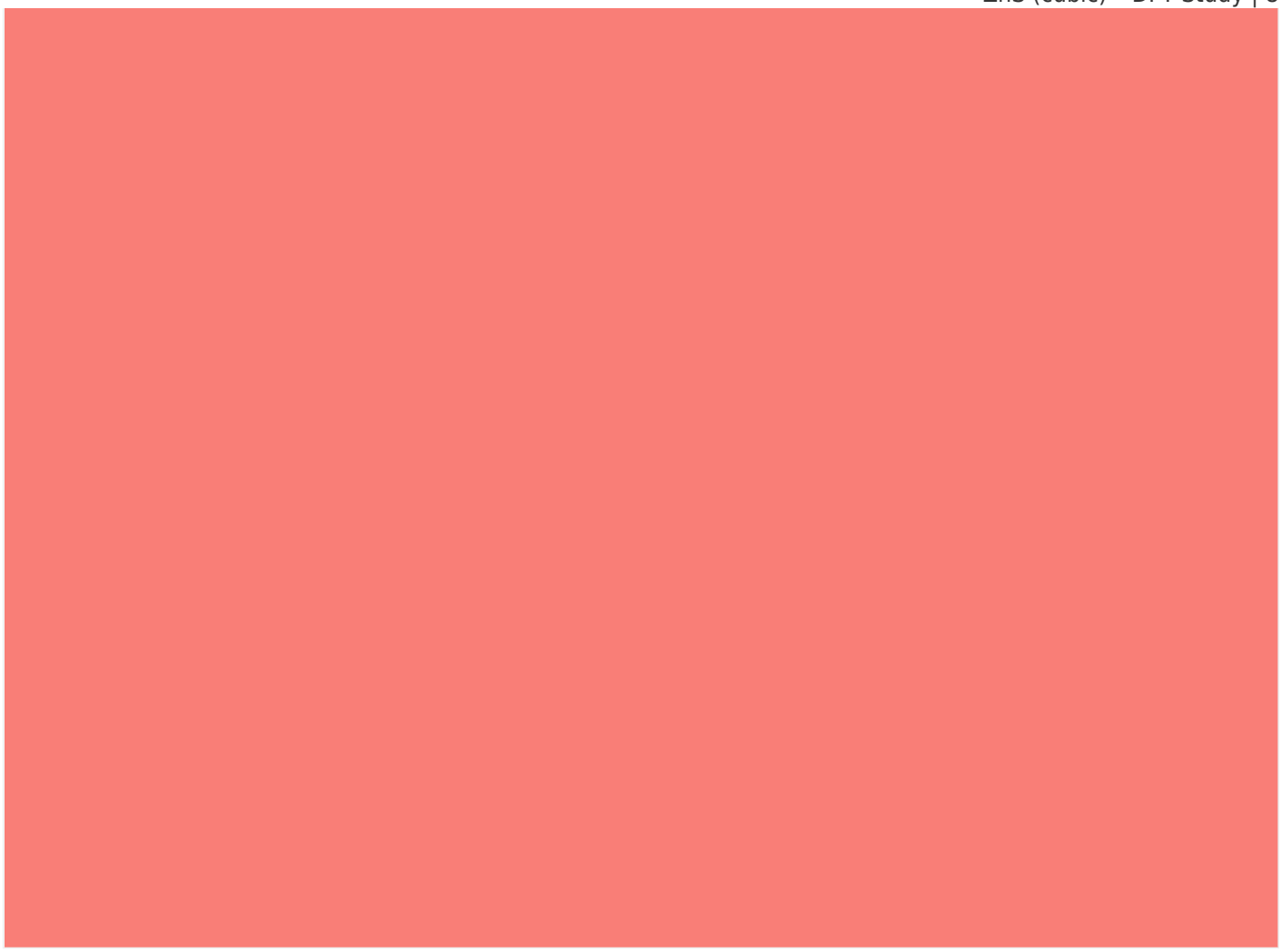

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