Crystal Structure:

CdS (Wurtzite)

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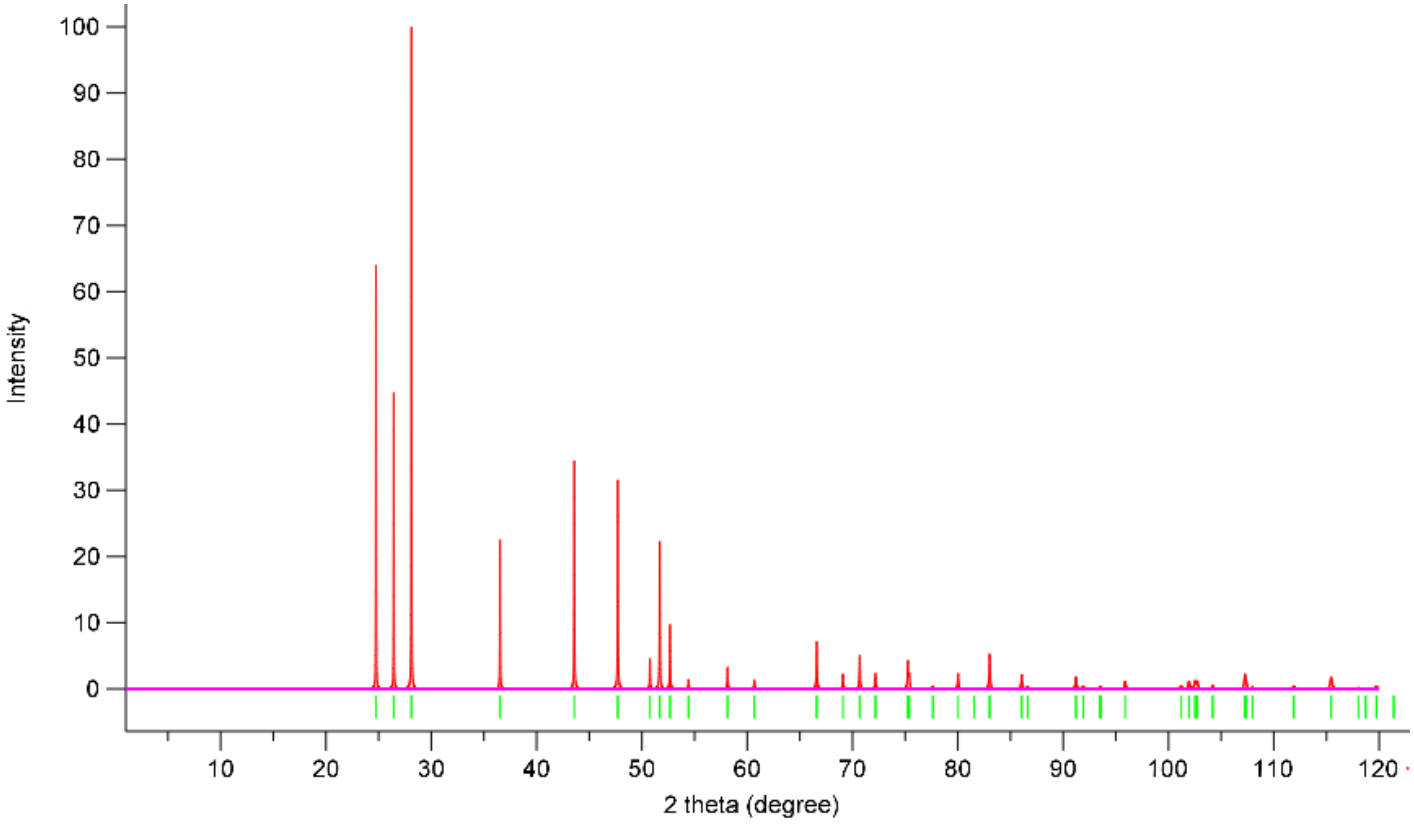
CIF Source:
Ulrich F, Zachariasen W
Zeitschrift fur Kristallographie 62 (1925) 260-273
Ueber die Kristallstruktur des alpha- und $-beta Cd S, sowie des Wurtzits.
_cod_database_code 1011054
_database_code_amcsd 0017955
http://rruff.geo.arizona.edu/AMS/download.php?id=12088.cif&down=cif

Simulated Powder XRD using VESTA:

X-Ray Wavelength: 1.54059 Angstrom



XRD Pattern Simulation of CdS (Wurtzite)

Simulation 1: GGA

Pseudopotential Used:
Cd.pbe-n-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: 40 Ry
Charge Density Energy Cutoff: 440 Ry
k – mesh: 8x8x8
Run Type: GGA-PBE

Total Energy vs Cutoff:

Cutoff(Ry)	Total Energy(Ry)
25	-242.21074772
30	-242.76744591
35	-242.82833344
40	-242.82984026
42	-242.83090181
45	-242.83403075
50	-242.83980923
55	-242.84302578

Optimized Coordinates and Lattice Parameters:

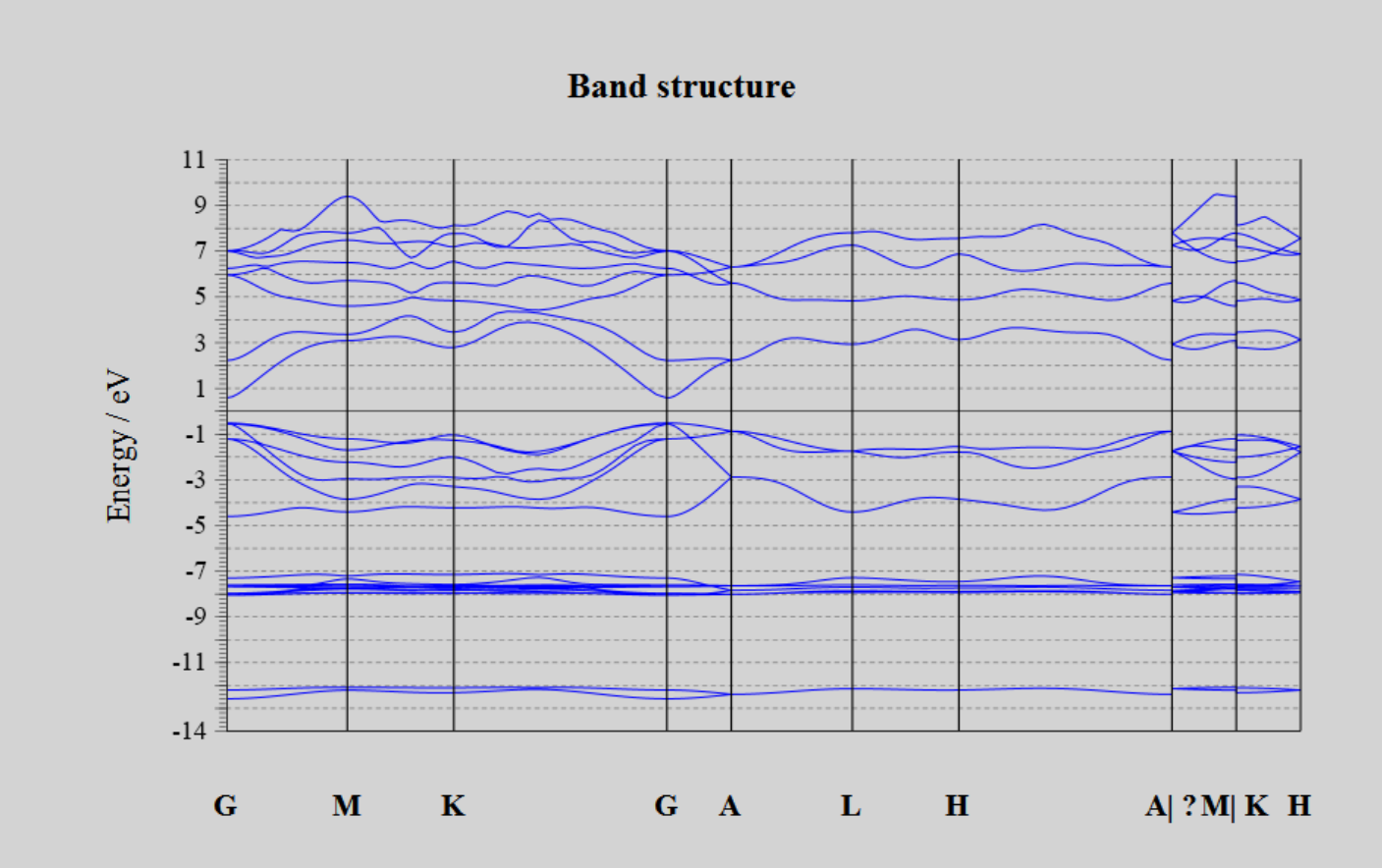
CELL_PARAMETERS {angstrom}

4.201514 0.000007 0.000001
-2.100751 3.638607 -0.000001
0.000001 -0.000002 6.842562

ATOMIC_POSITIONS {angstrom}

Cd1 -0.000009 2.425756 6.838208
Cd1 2.100752 1.212894 3.416927
S1 -0.000008 2.425757 2.570314
S1 2.100752 1.212891 5.991596

Bandstructure:

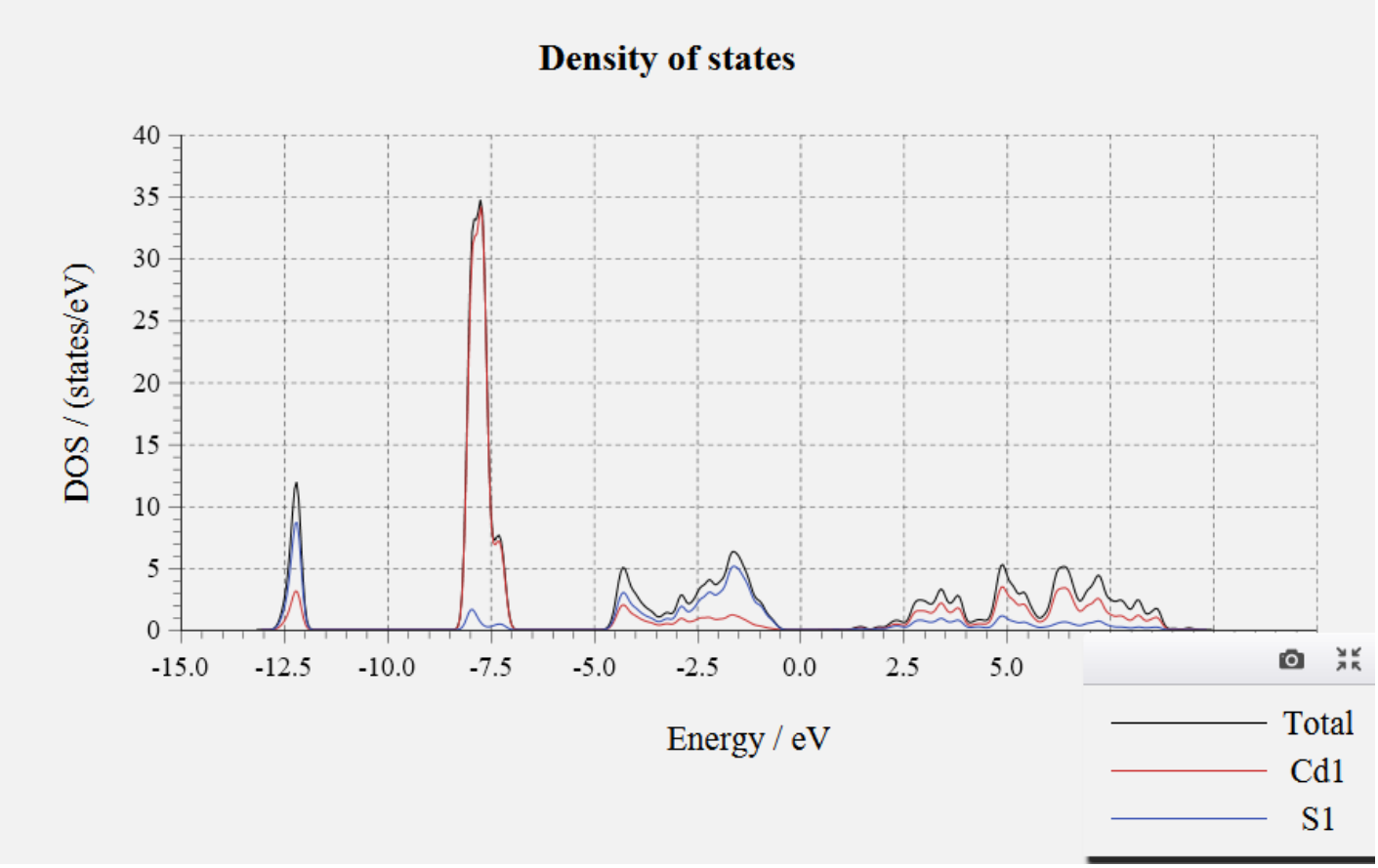


Bandstructure along high symmetry points of CdS (Wurtzite)

highest occupied, lowest unoccupied level (ev): 4.9390 6.0375

Band-gap: 1.0985 eV

Density of States(DOS):



Total and projected density of states (DOS) of CdS Wurtzite

Input Files:

CdS (wurtzite) 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

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

http://www.sciencedirect.com/science/article/pii/S0038109814000775

http://iopscience.iop.org/article/10.1088/1674-4926/38/7/073001/meta

http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.752.8420&rep=rep1&type=pdf

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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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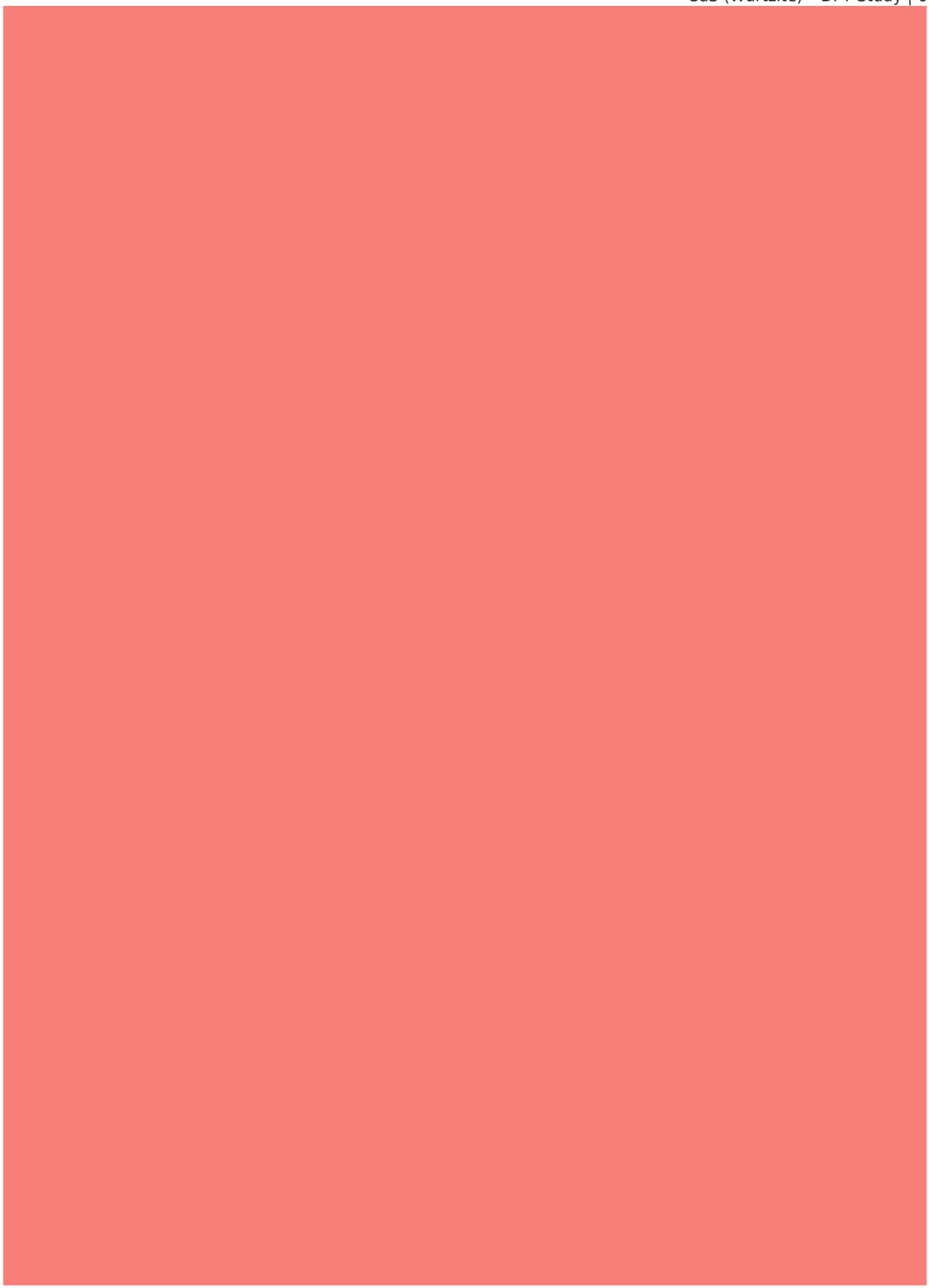

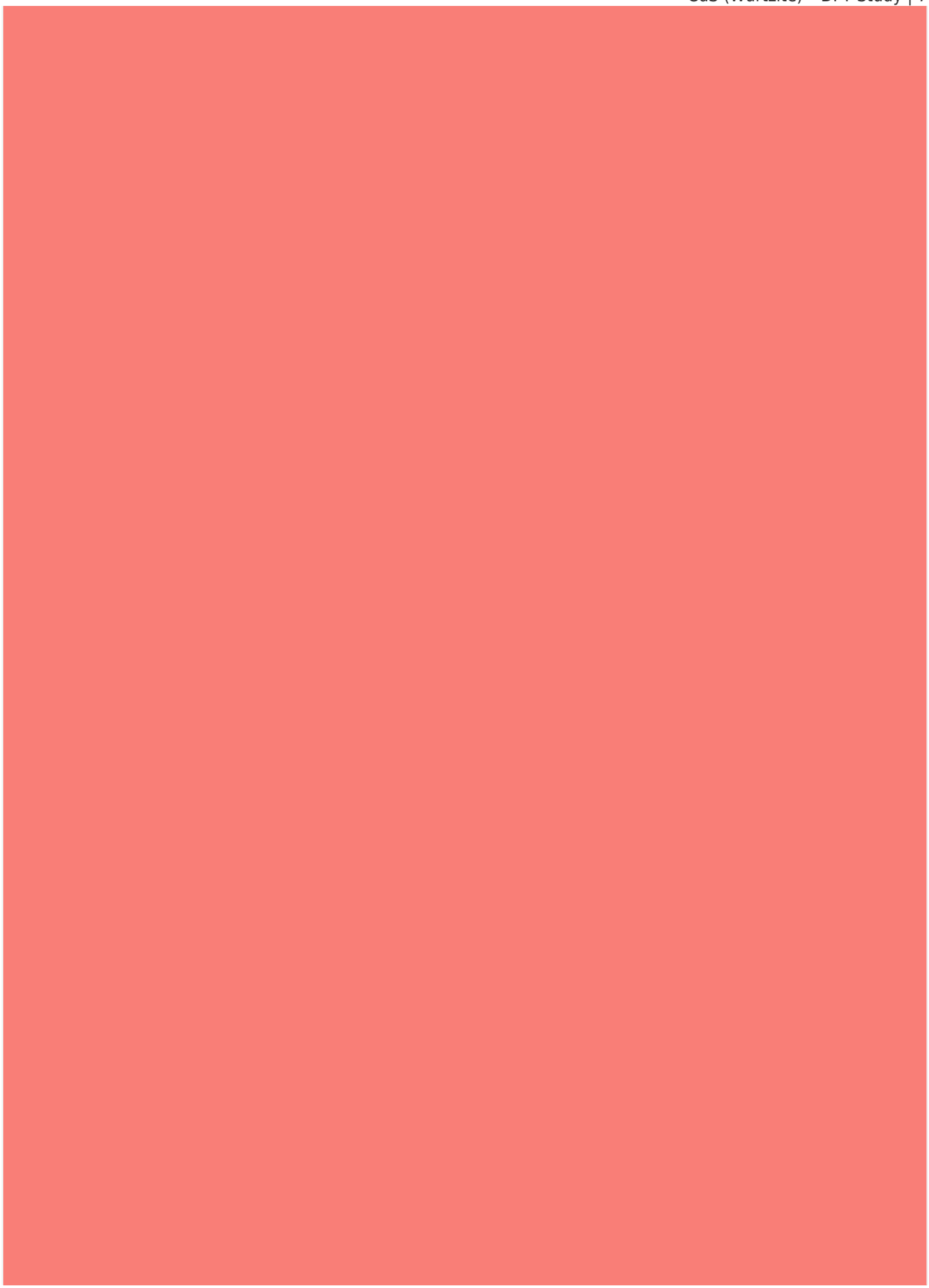

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