

Crystal Structure:

Ni (FCC)

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CIF Source:

Wyckoff R W G

Crystal Structures 1 (1963) 7-83

Second edition. Interscience Publishers, New York, New York

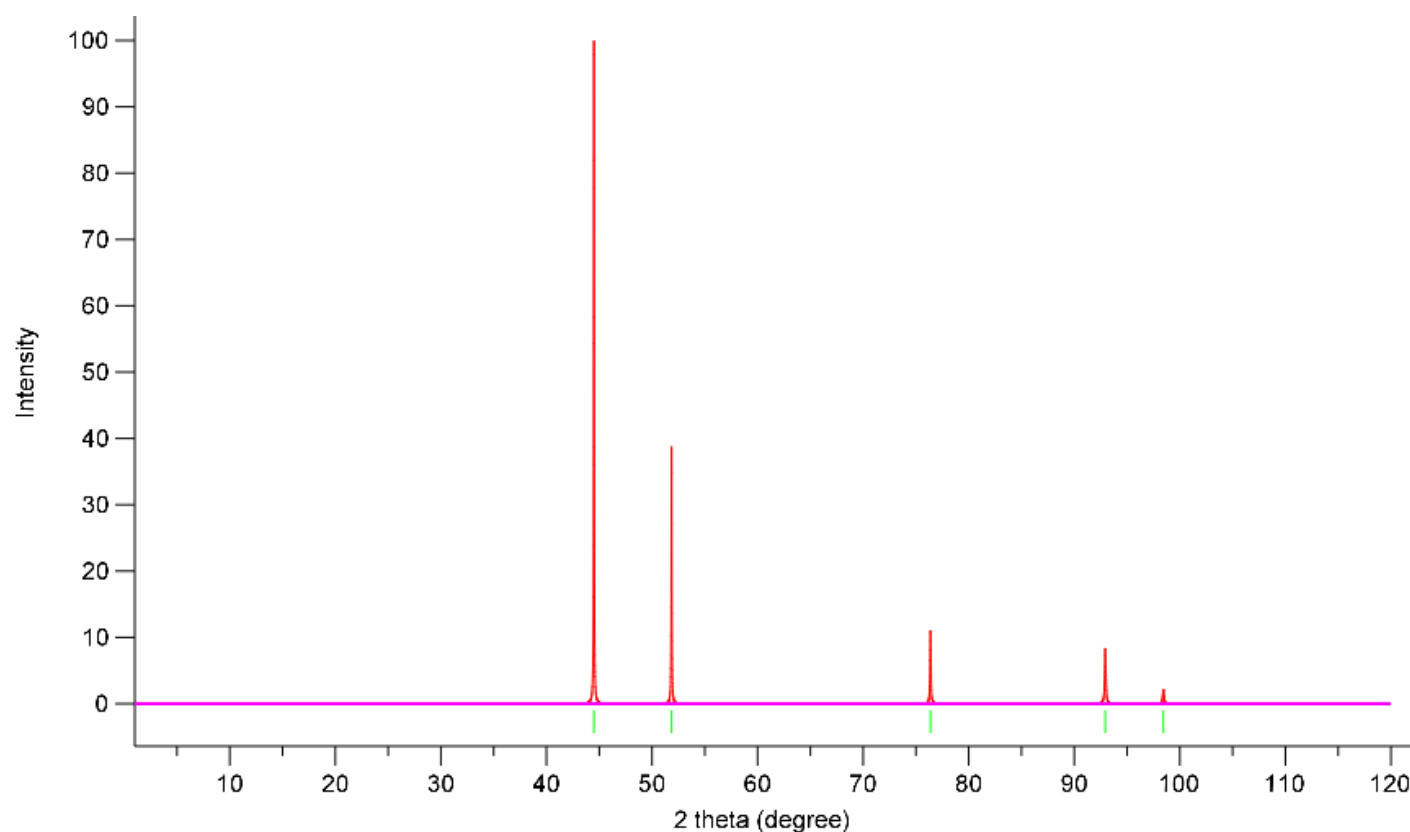
Cubic closest packed, ccp, structure

_database_code_amcsd 0011153

<http://rruff.geo.arizona.edu/AMS/download.php?id=13141.cif&down=cif>

Simulated Powder XRD using VESTA:

X-Ray Wavelength: 1.54059 Angstrom



Nickel (Ni-FCC) Powder XRD Pattern Simulation using VESTA

Simulation 1: GGA-Spin Polarized

Pseudopotential Used:

Ni.pbe-n-rrkjus_psl.1.0.0.UPF

PP Type: Ultrasoft

Exchange Correlation Functional: PBE-GGA Spin Polarized

Non-linear core corrections are used.

Wavefunction Energy Cutoff: 42 Ry
 Charge Density Energy Cutoff: 462 Ry
 k – mesh: 8x8x8
 Run Type: GGA-PBE
 Starting Magnetization: 0.8

Total Energy vs Cutoff:

Cutoff(Ry)	Total Energy(Ry)
25	-401.99506705
30	-402.27359712
35	-402.29449826
40	-402.29684732
42	-402.29943963
45	-402.30405077

In order to perform spin polarized calculations set the `nspin` parameter to 2.

Then as explained [here](#), set a starting magnetization to break the symmetry. The calculation should find the lowest-energy spin state compatible with the given crystal structure and not orthogonal to initial conditions (e.g.: if you start with a FM alignment, you will hardly find an AFM final state even if it exists). Perform several calculations at different starting magnetizations, choose the one with smaller energy as ground state. The system must be in all cases treated as a metal, whether it is or not. In principle, you should use pseudopotentials with the nonlinear core correction.

The following shows the total energy for different values of starting magnetization. NOTE: Starting magnetization is given in fractions, ranging between -1 (all spins down for the valence electrons of atom type 'i') to 1 (all spins up).

Total Energy vs Starting Magnetization:

SM	Total Energy (Ry)	Tot. Magnetic Mom/Abs. Mg. Mom. (Bohr Magneton)
0.1	-402.29944015	2.45/2.78
0.2	-402.29943963	2.45/2.78
0.3	-402.29944012	2.45/2.79
0.4	-402.29944012	2.45/2.79
0.5	-402.29943998	2.45/2.78
0.6	-402.29944016	2.45/2.78
0.7	-402.29943952	2.45/2.79
0.8	-402.29944019	2.45/2.78
0.9	-402.29944019	2.45/2.78
1.0	-402.29944012	2.45/2.78

Clearly, a starting magnetization value of 0.8 gives the lowest energy.

Now, we perform optimization of geometry.

Optimized Coordinates and Lattice Parameters:

CELL_PARAMETERS {angstrom}

3.510370	0.000000	0.000000
0.000000	3.510370	0.000000
0.000000	0.000000	3.510370

ATOMIC_POSITIONS {angstrom}

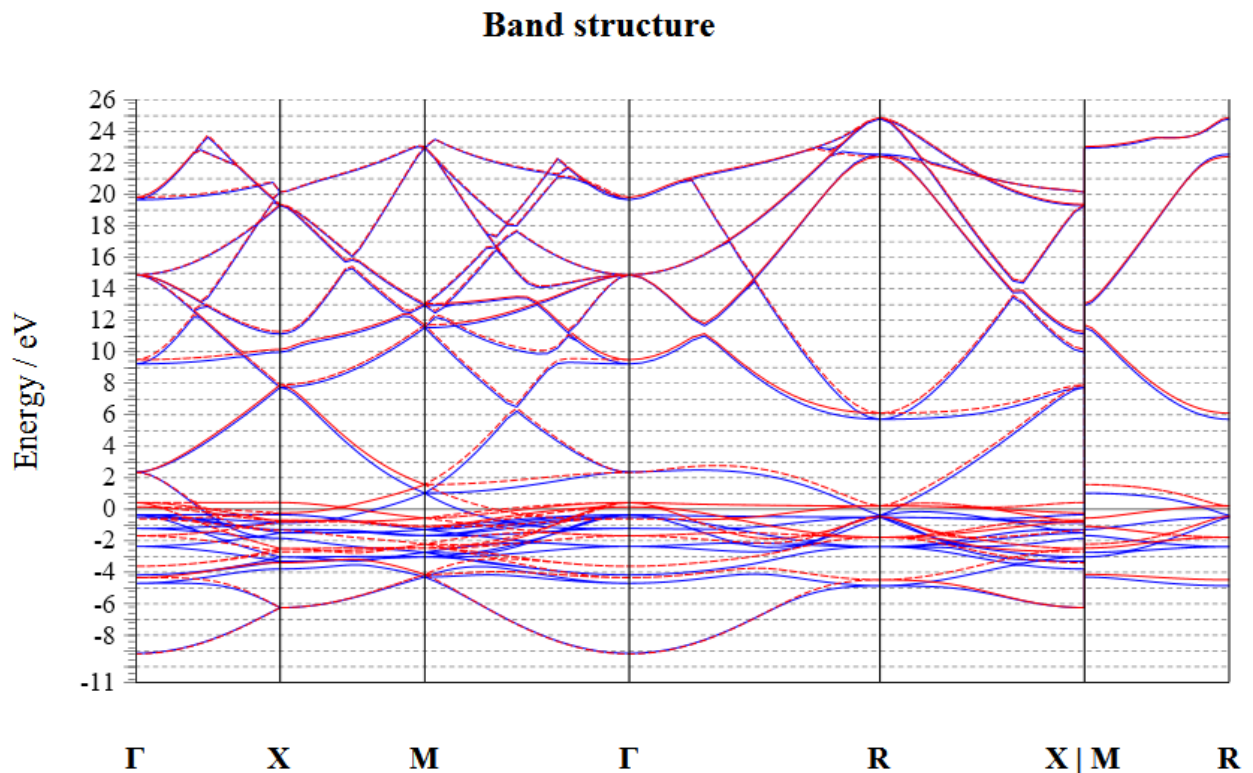
Ni	0.000000	0.000000	0.000000
Ni	0.000000	1.755185	1.755185
Ni	1.755185	0.000000	1.755185
Ni	1.755185	1.755185	0.000000

Total magnetic moment for optimized system: 2.43 Bohr Magneton.

Since there are 4 Ni atoms in our FCC lattice, therefore, the total magnetization per atom is $2.43/4=0.6075$ Bohr. Magnt. which is astoundingly very close to the experimental value of 0.6 B.M.

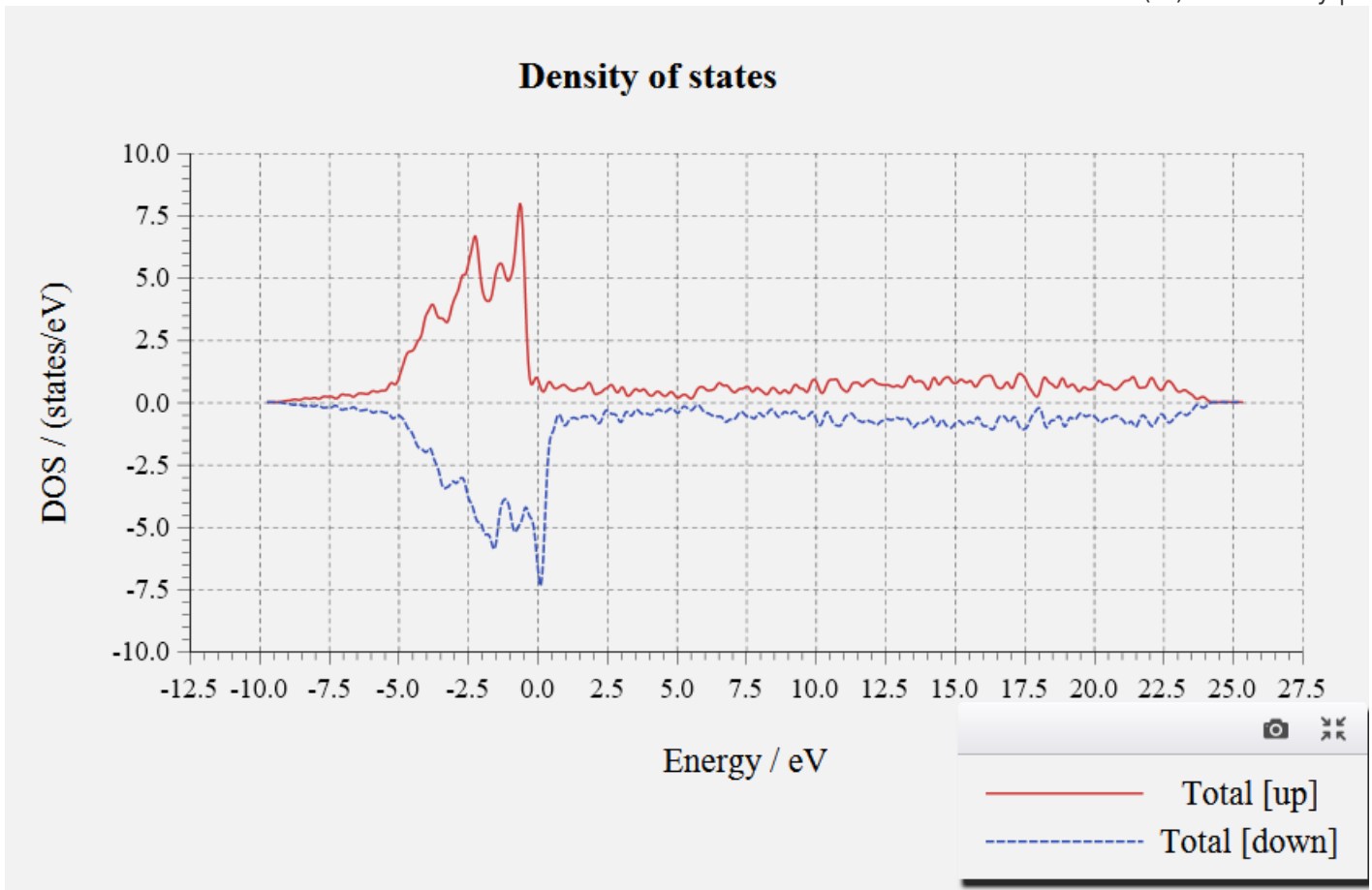
Magnetic moment per atom= 0.6075 B.M.

Bandstructure:



Bandstructure of Ni(FCC) along high symmetry points

Density of States(DOS):



Density of states of Ni

Input Files:

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/>

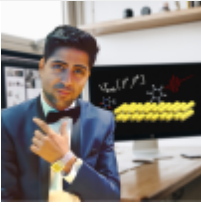
References and Resources

https://www.researchgate.net/figure/263203110_The-density-of-states-DOS-states-atom-eV-of-paramagnetic-nickel-in-which-there-are

<http://www.materialsdesign.com/appnote/magnetic-moment-iron>

<http://www-rjn.physics.ox.ac.uk/lectures/magnetismnotes10.pdf>

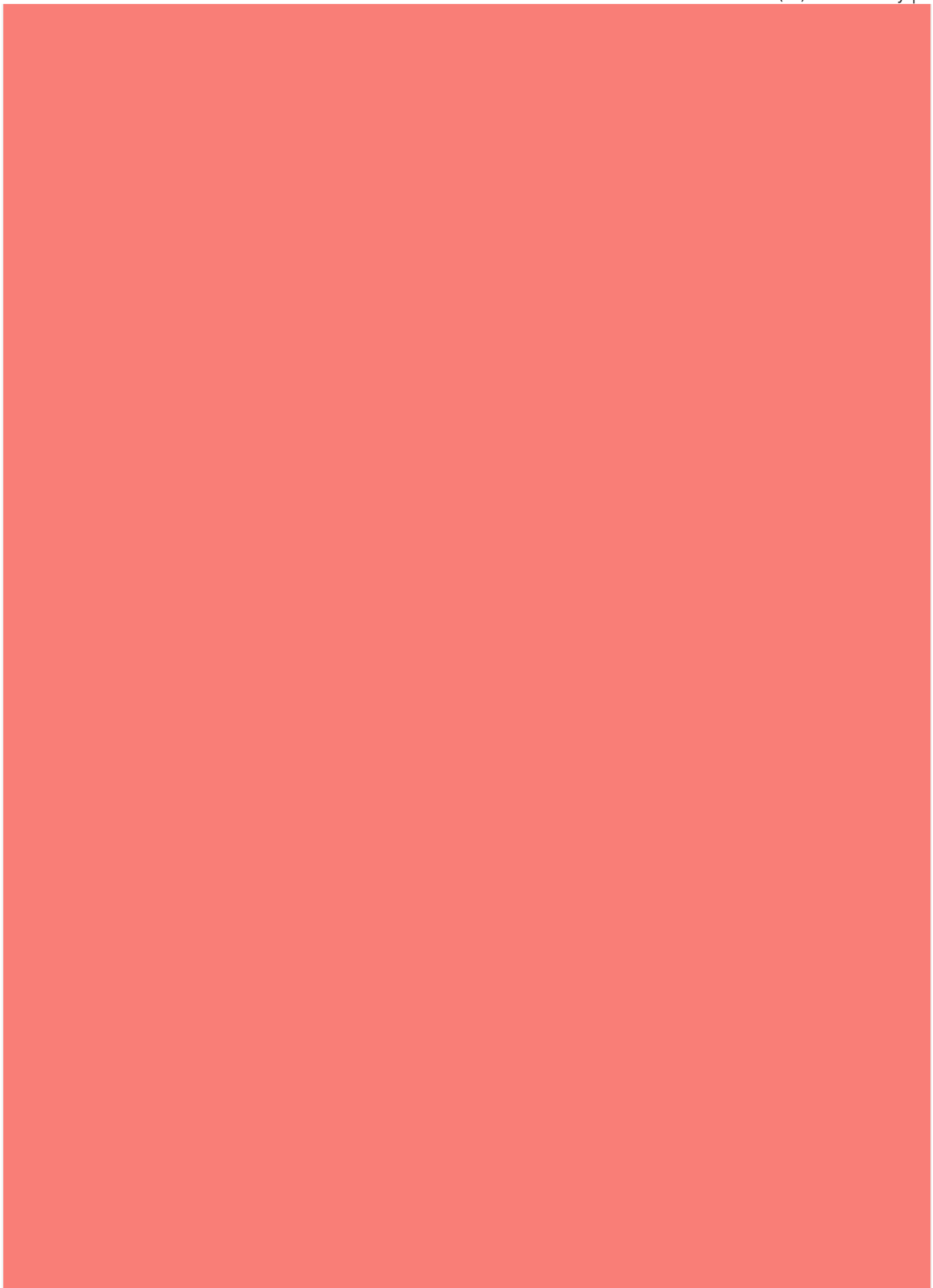
<http://146.141.41.27/Lectures/Omololu-Wednesday-21-MetalsMagnetism2.pdf>

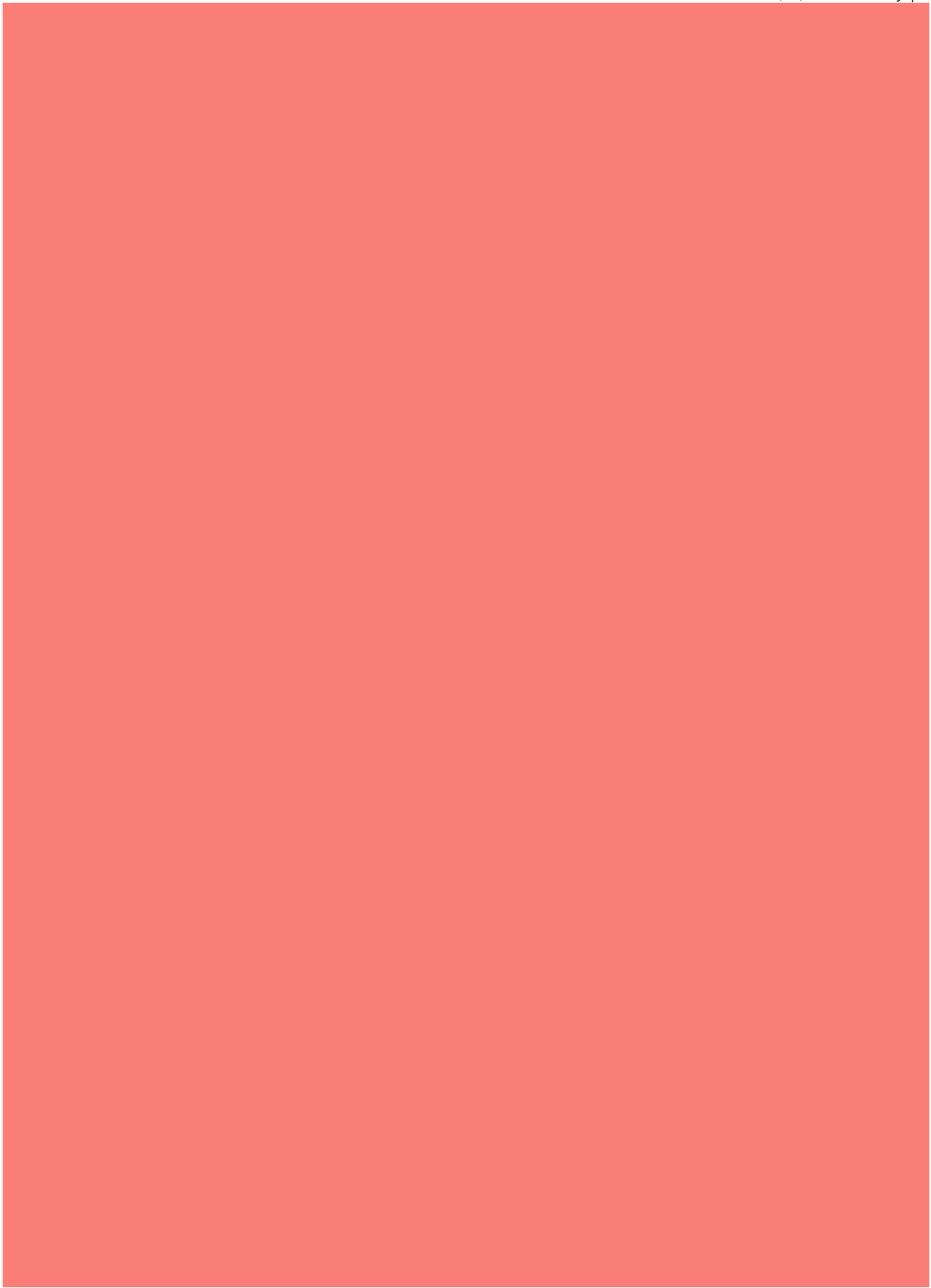


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I'm a physicist specializing in computational material science with a PhD in Physics from Friedrich-Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, 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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