

Chemical File Format Converter

The following is the Web Application built using Python, [Open Babel](#), [Py3Dmol](#) and [Streamlit](#) that allows inter-conversion between various [chemical file formats](#) in current use.

Web App

You can also open this [link](#) to go full screen.

Your browser does not support iframes.

Currently, the web app supports converting to and from the following chemical file formats:

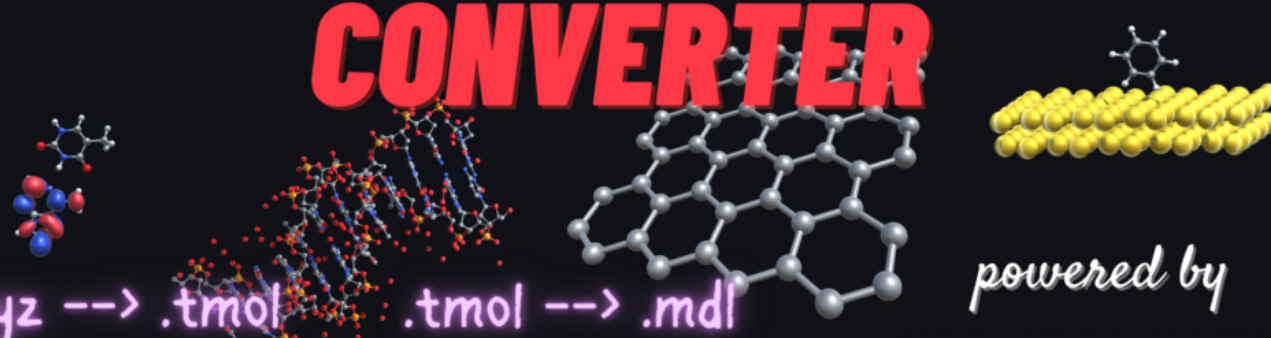
Input

- xyz
- tmol – Turbomole coord format
- sdf
- cif
- poscar
- cube
- fhiaims
- mcif
- mdl
- mol
- mol2
- outmol
- pwscf
- smi
- pdb
- smiles

Output

- xyz
- tmol – Turbomole coord format
- sdf
- cif
- cube
- fhiaims
- mcif
- mdl
- mol
- mol2
- outmol
- smi
- pdb
- smiles

CHEMICAL FILE FORMAT CONVERTER



powered by

OPEN BABEL
&
PY3DMOL

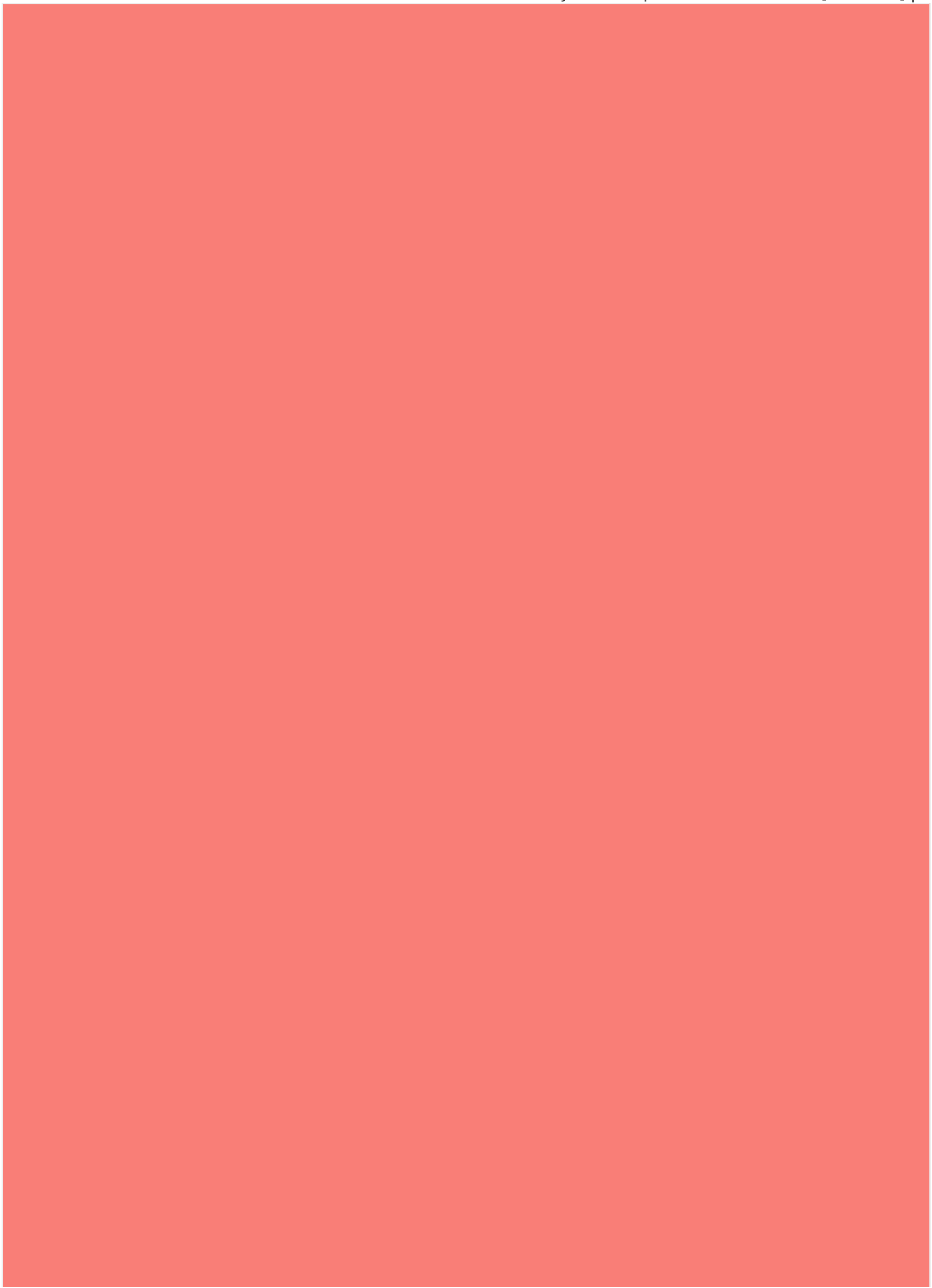
`.xyz --> .tmol` `.tmol --> .mdl`
`.pdb --> .mol` `smiles --> .txyz`
`.pwscf --> .cif` `.cub --> fhiaims`
`.mcif --> .sdf` `.poscar --> .cif`

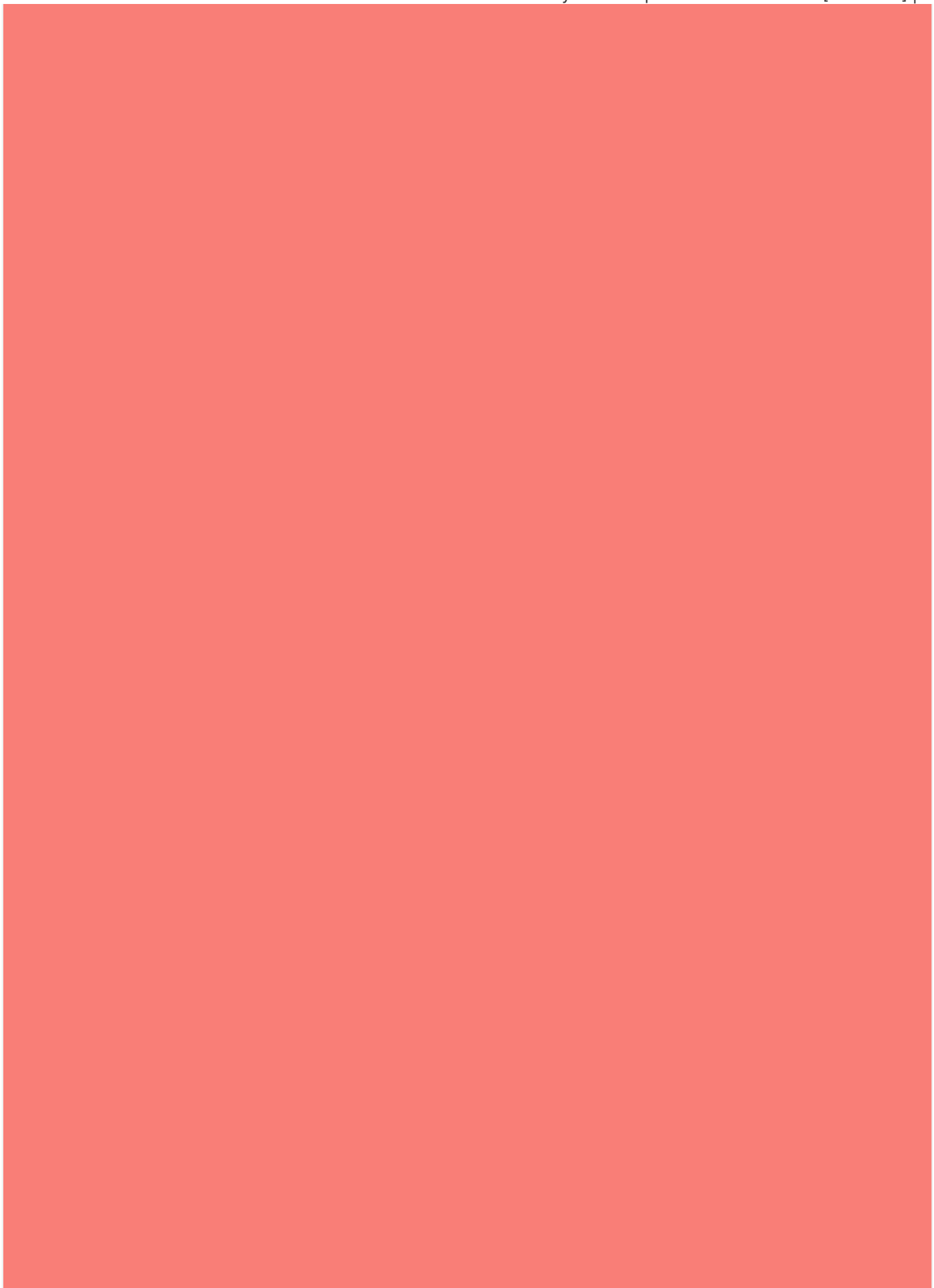


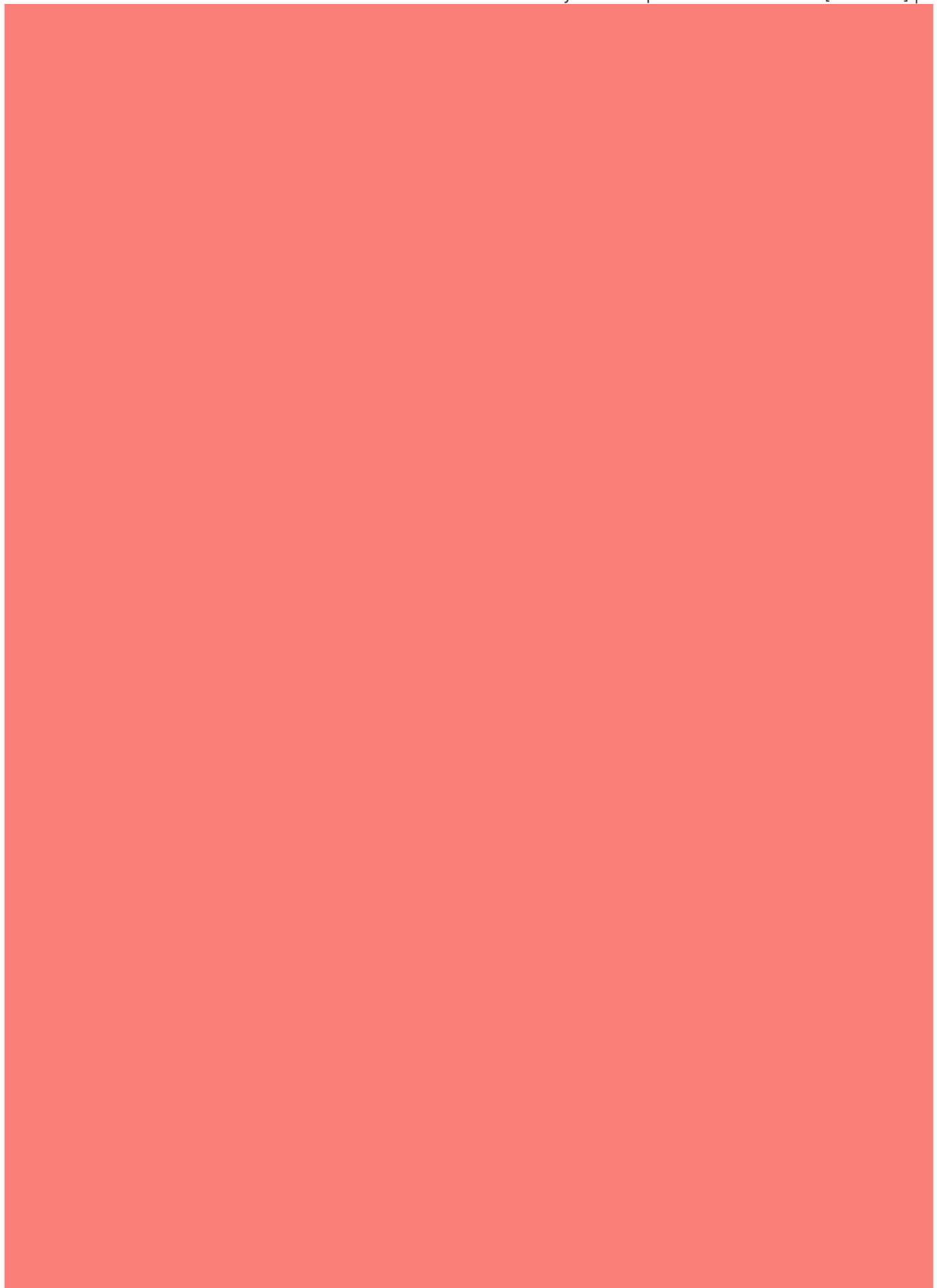
Manas Sharma

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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