The following is the Web Application built using Python, BSE and Streamlit that allows inter-conversion between various basis set formats used by different Quantum Chemistry Softwares.

Web App

You can also open this link to go full screen.

The main motivation behind creating the tool was to convert the Crystal basis sets and ECPs to Turbomole format. Most of the commonly used basis sets can already be found in various formats at the https://www.basissetexchange.org/, with the exception of Crystal basis sets.

Crystal basis sets can be found at this link: https://www.crystal.unito.it/basis-sets.html

The user can then copy a particular basis set and paste it in the web app to convert it to Turbomole format.

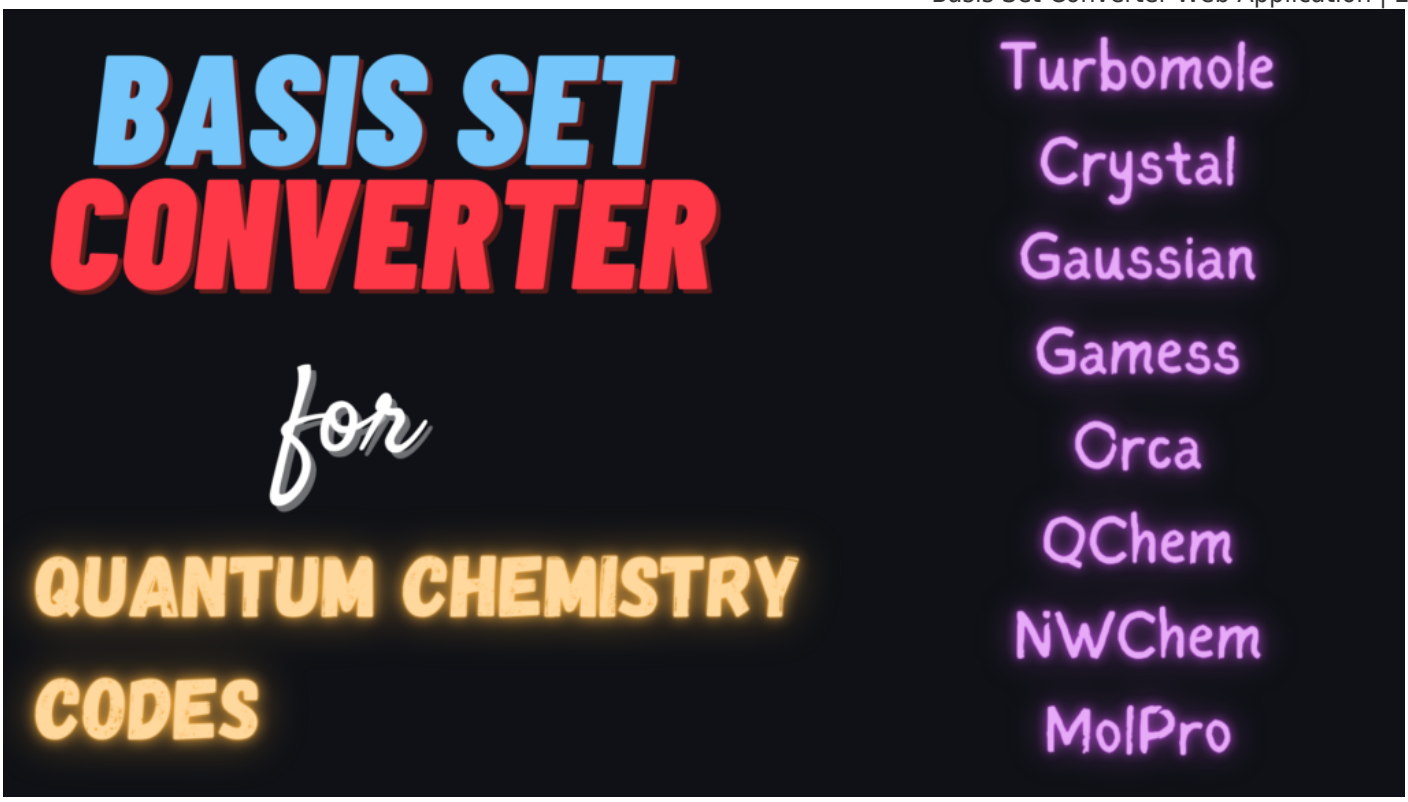
Warning: During testing, it was discovered by Prof. Sierka, that for pob-XVZ basis sets, the ECPs provided in the original publications contain different exponents of the r factors than expected by TURBOMOLE. Essentially, these factors were found to be reduced by 2, resulting in 0 instead of 2, 2 instead of 4, and so on. For proper usage of the ECPs provided with the pob-XVZ basis sets in TURBOMOLE, one should therefore increase the exponent of the r factors by 2 if the basis sets were obtained from the official publications. The next version of TURBOMOLE, i.e., 7.8 should come with pob-TZVP-rev2 and pob-DZVP-rev2 basis sets included with the corrected ECPs.

Supported formats:
1. *Turbomole*
2. *Crystal*
3. *MolPro*
4. *QChem*
5. *NWChem*
6. *Orca*
7. *Gaussian*
8. *Dalton*

The tool/web app was created in the group of Prof. Dr. Marek Sierka, by Manas Sharma.

For more details relating to code, please refer to the GitHub repo:
https://github.com/manassharma07/Basis_Set_Format_Converter

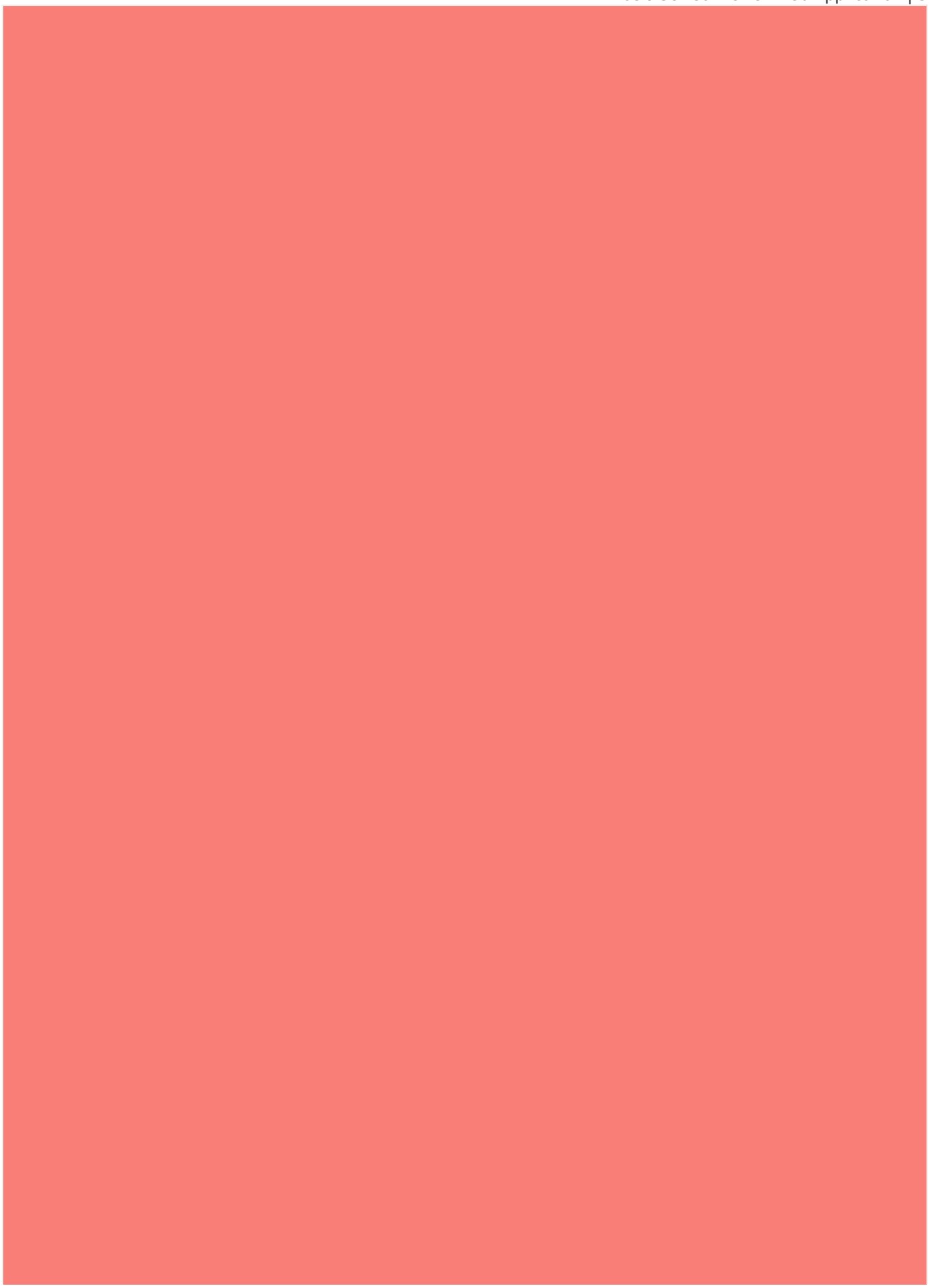
YouTube Tutorial

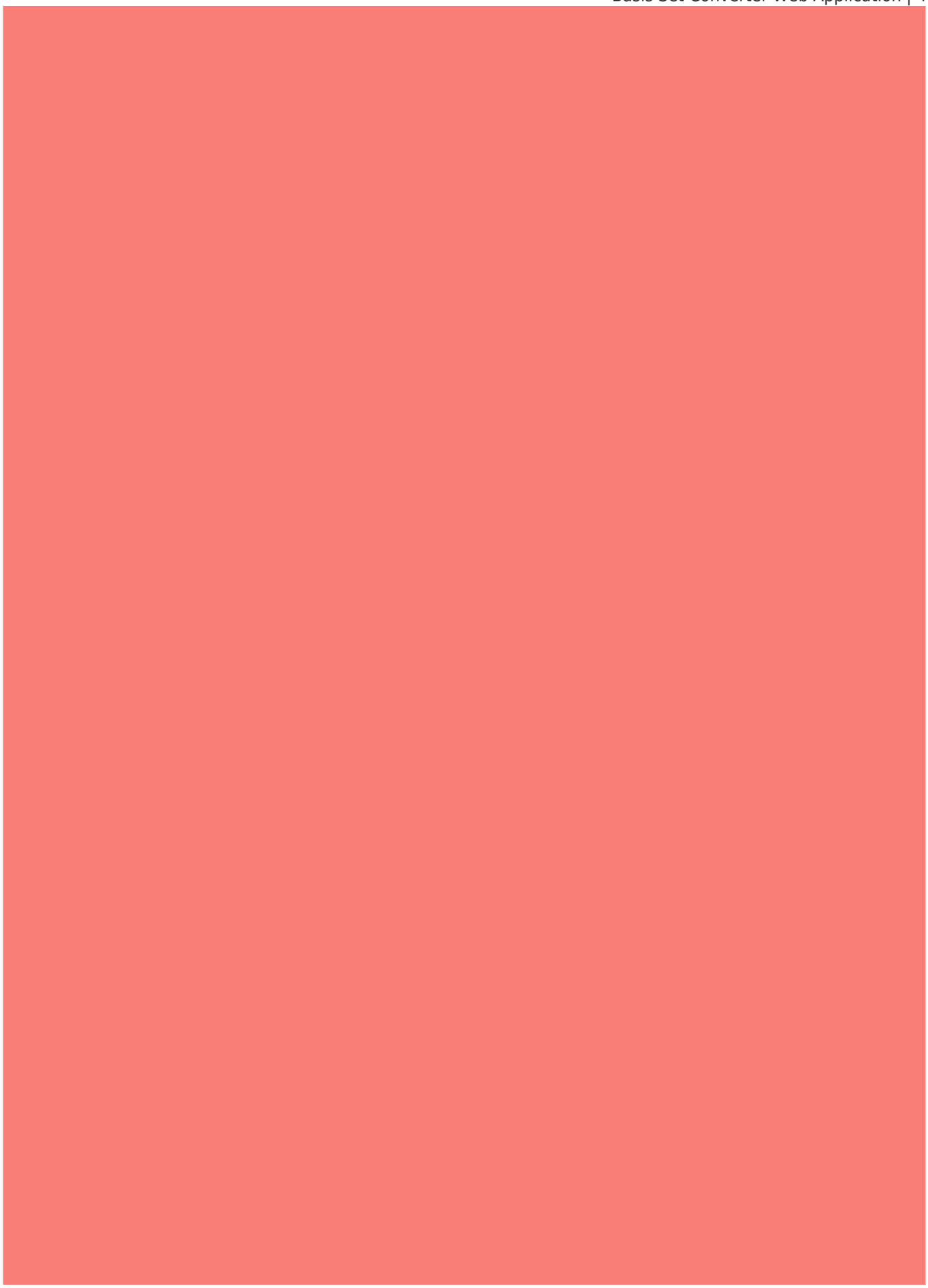


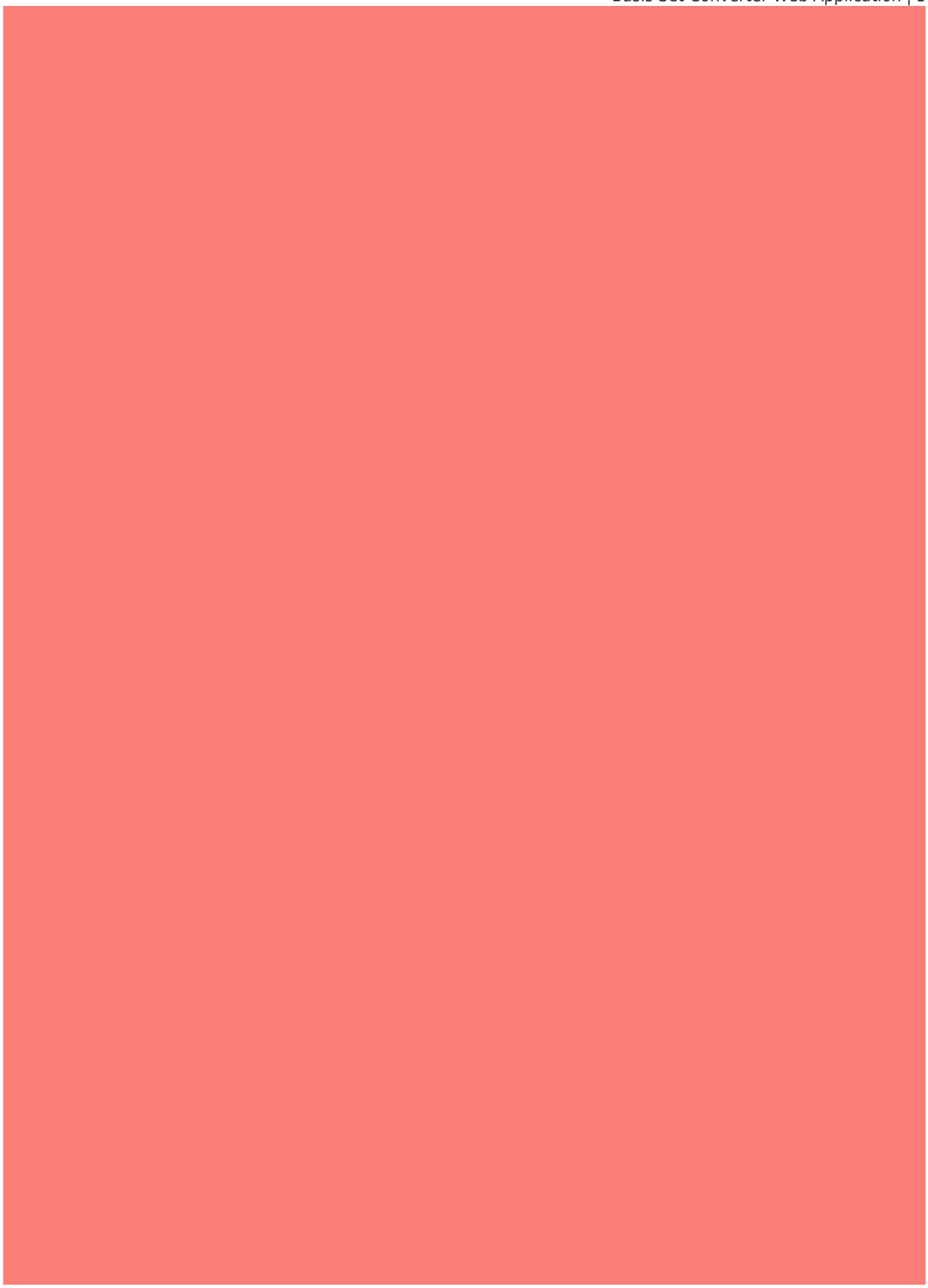
Manas Sharma

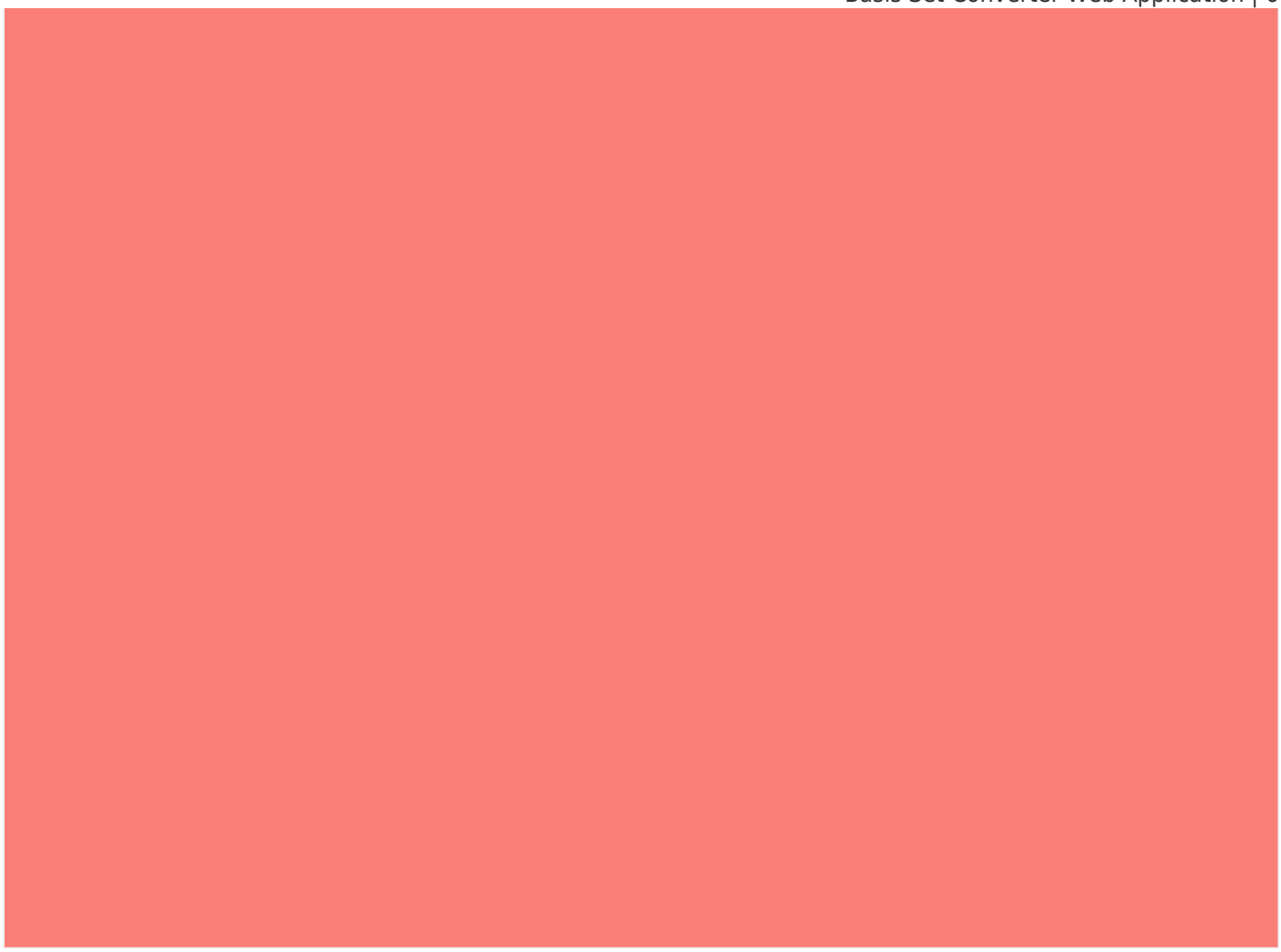
I’m a physicist specializing in computational material science with a PhD in Physics from Friedrich-Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, and Machine Learning related apps and software from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