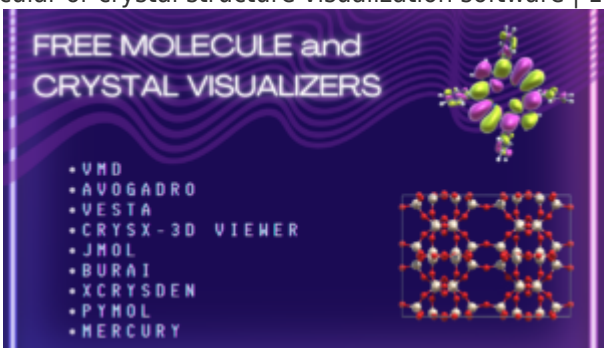
When I first got into density functional theory (DFT) calculations (in 2017), the first crystal structure visualizer I used was BURAI (which is a GUI for Quantum ESPRESSO).




Soon, I also started using VESTA, which is an excellent application that has been in development for years and offers a wide variety of features.

However, as I got further into computational material science I got to use many more amazing applications each with its own unique features. In fact, I even developed my own molecule and crystal visualization application (CrysX-3D Viewer) built using the Unity gaming engine that works on PCs and Android smartphones.

In this post, I will try to make a list of some of the *notable* yet free visualization applications that are currently available in the market.

Please note: The order in which I recommend the programs is not indicative of their ranking or quality.

# 1. VESTA

VESTA is a 3D visualization software for structural models, crystals, and electron density. Some of its key features include:

- Support for various structural formats, such as CIF, POSCAR, XYZ, CUBE, and more.
- Multiple visualization modes, including space-filling, stick, ball-and-stick, and wireframe.
- Customizable color schemes and rendering styles, allowing users to highlight specific elements or structures.
- Advanced measurement tools, such as distance, angle, and torsion angle calculations.
- Synthetic crystal generation, allowing users to create and visualize hypothetical structures.
- Extended modeling and analysis capabilities for DFT calculations.
- Powder X-Ray diffraction simulator.
- Multilingual support, with interface available in English, Japanese, and Chinese.
- Cross-platform compatibility, with versions available for Windows, Mac, and Linux.
- Extensive documentation and tutorials, providing users with a comprehensive guide to using the software.

I have created some tutorials on VESTA that you can watch here.

# 2. BURAI

- BURAI is a graphical user interface (GUI) for Quantum ESPRESSO (QE).
- Although it was mainly created to offer a user-friendly interface for setting up, running, and analyzing QE calculations, it can also be used as a visualizer for .CIF, .XYZ and QE input files.
- My favorite is the capability to intuitively model supercells, monolayers, and defects.
- It also allows users to easily modify input parameters for various calculations.
- BURAI also provides useful graphical representations of simulation results, including total energy, density of states, and band structures.
- It can be used on Windows, macOS, and Linux operating systems. Please note: For me, it worked seamlessly only on Windows. I had trouble running QE calculations on Macs and in launching the visualizer on Linux.
- BURAI is developed and maintained by a team of researchers at the Department of Materials Engineering, Kyushu University, Japan.

I have created some tutorials on BURAI that you can watch here.

# 3. JMOL

- JMOL is a free, open-source molecular visualization program.
- It allows users to view and manipulate 3D models of small molecules and macromolecules, such as proteins and nucleic acids.
- JMOL can read a variety of file formats, including PDB, CIF, CUBE, MOL, and XYZ, and can display a wide range of molecular properties, such as atomic positions, bond distances, densities, orbitals, and charges.
- It offers a number of visualization options, including different color schemes and representations (e.g. ball-and-stick, space-filling), as well as a range of animation tools to generate movies of molecular dynamics.
- JMOL can be used on Windows, Mac, and Linux operating systems.
- It is developed and maintained by an active community of researchers and developers, and is regularly updated with new features and improvements.
- My personal favorite are the scripting capabilities, which allow users to automate repetitive tasks and create custom scripts for specific purposes. This can be useful for generating large numbers of images or animations, or for analyzing data in a more efficient and systematic way. Users can access the JMOL scripting language through the program's built-in scripting console, or by using external text editors and running the scripts directly within JMOL. The scripting language is based on the popular Java programming language, and offers a range of commands and functions for manipulating and analyzing molecular data. JMOL also has a number of built-in scripts and tools, such as the Jsmol Applet, which allows users to embed interactive molecular models in web pages and other online platforms. This can be useful for creating educational resources or sharing research findings with a wider audience. In fact, this website also uses Jsmol in several places to give an interactive visualization of chemical systems.

I have created some tutorials on BURAI that you can watch here.

# 4. CRYSX SUITE (3D VIEWER, AR, and CRYSTALLOGRAPHIC TOOLS)

I have developed a suite of applications useful for real-time high-quality visualization of molecules and crystals under the CrysX brand.

## CRYSX-3D VIEWER

- CrysX-3D Viewer is built using the Unity gaming engine.
- The main advantage of CrysX-3D Viewer over other visualizers is the advanced shaders (from Unity) used to visualize the chemical systems.
- Due to the aesthetically appealing visualization quality combined with lighting and shadow capabilities offered by Unity, it is best used for creating graphical abstracts/TOCs, figures, and covers for your manuscripts.
- CrysX-3D Viewer is available on Windows, Linux, MacOS, and Android.
- CrysX-3D Viewer can export images of the molecules and crystals as transparent PNGs, which is quite useful when making figures for PowerPoint slides or Posters with colored backgrounds.
- Supports .MOL, .XYZ, .CIF and .CUBE (for densities and orbitals) formats.
- It is the only application that offers a smartphone version, albeit only for Android.
- Has a variety of effects like ambient occlusion, bloom, and particle effects.
- Ball-and-stick and wireframe visualization modes for structures.
- Can visualize Miller/lattice planes.
- As its developer, I would also like you to know about some of its limitations. One major problem is that some features related to exporting and modeling may not work, even if there is a button that says otherwise. I'm

trying my best to improve the shortcomings soon.

### CRYSX-AR

- CrysX-AR can visualize molecular and crystal structures in augmented reality.
- CrysX-AR is only available for Android smartphones.
- It is powered by Google ARCore engine.
- Supports .XYZ, .MOL, and .CIF formats.

### Other relevant apps in CrysX suite

In addition to CrysX-3D Viewer and CrysX-AR, there are some visualization capabilities in CrysX-Crystallographic Tools (Android app) and CrysX-CompChem File Converter web application.

CrysX-Crystallographic Tools has features like a powder X-Ray diffraction simulator, space group decoder, experimental XRD analyzer, file converter, periodic table, etc.

CrysX-CompChem File Converter can be used to interconvert between various file formats used in computational material science and also visualize the molecular structures.

I have created some tutorials on CrysX that you can watch here.

## 5. AVOGADRO

- Avogadro is a free, open-source molecular visualization and analysis program.
- It allows users to view, manipulate, and analyze 3D models of small molecules and macromolecules, such as proteins and nucleic acids.
- Avogadro can read a variety of file formats, including PDB, CIF, and XYZ, and can display a wide range of molecular properties, such as atomic positions, bond distances, and charges.
- It offers a number of visualization options, including different color schemes and representations (e.g. ball-and-stick, space-filling), as well as a range of animation tools.
- Avogadro can be used on Windows, Linux and MacOS
- It is developed and maintained by an active community of researchers and developers, and is regularly updated with new features and improvements.
- Avogadro offers a number of extensions for quantum chemistry programs, such as ORCA.
- These extensions allow users to create input files for quantum chemistry calculations directly within Avogadro, and to visualize and analyze the results in a convenient and intuitive way.
- Avogadro also provides tools for visualizing and analyzing the results of quantum chemistry calculations, such as plotting energy levels and orbital populations, and calculating and visualizing molecular orbitals.

## 6. VMD

- VMD (Visual Molecular Dynamics) is a free, open-source program for visualizing and analyzing biomolecular systems.
- It allows users to view and manipulate 3D models of proteins, nucleic acids, and other biomolecules, as well as their interactions with small molecules and other biomolecules.
- VMD can read a variety of file formats, including PDB, CIF, and XYZ, and can display a wide range of molecular properties, such as atomic positions, bond distances, and charges.
- It offers a number of visualization options, including different color schemes and representations (e.g. ball-and-stick, space-filling), as well as a range of animation tools.
- VMD can be used on Windows, Linux and MacOS.
- Personally, I am not a fan of the antiquated GUI but it gets the job done so no complaints.

- Has a variety of settings to generate high quality renders for manuscripts and journal covers, albeit not in real-time.
- It is developed and maintained by an active community of researchers and developers, and is regularly updated with new features and improvements.
- VMD also offers scripting capabilities, which allow users to automate repetitive tasks and create custom scripts for specific purposes. This can be useful for generating large numbers of images or animations, or for analyzing data in a more efficient and systematic way.

# 7. XCRYSDEN

- XCrySDen is a free, open-source crystalline and molecular visualization program.
- It allows users to view and manipulate 3D models of crystals, molecules, and other periodic structures, such as surfaces, interfaces, and defects.
- XCrySDen can read a variety of file formats, including PDB, XSF (its own format), and XYZ, and can display a wide range of structural properties, such as atomic positions, bond distances, and lattice vectors.
- It offers a number of visualization options, including different color schemes and representations (e.g. ball-and-stick, space-filling), as well as a range of animation tools.
- XCrySDen can be used on Windows, MacOS and Linux.
- In addition, it can visualize chemical structures for the following ab initio simulation software:
  Quantum ESPRESSO
  WIEN2k
  CRYSTAL
  GAUSSIAN
  Orca
  FHI98MD
- For crystal structures, it has the ability to:
  (a) switch between primitive and conventional cell settings;
  (b) change the number of the displayed unit cells, that is, display smaller or larger portions of a crystal;
  (c) display the crystal lattice;
  (d) visualize the Wigner-Seitz cell and Brillouin zone;
  (e) provide k-path selection for band-structure calculations;
  (f) visualize Fermi surfaces

# 8. PYMOL

- PyMOL is a user-sponsored molecular visualization system on an open-source foundation, maintained and distributed by Schrödinger.
- Its key feature is that it is built on top of a python backend and can be used for scripting.
- It offers a powerful and flexible interface with GUI and command line options.
- Although, it was conceived with biological systems in mind, it is relevant for any molecular system.
- While it is a commercial product, it is built on an open-source foundation and is available for free for Educational-Use-Only.
- PyMol can be installed with conda and is available on Windows, MAC, and Linux.

# 10. MERCURY

Mercury is a specialized software to treat/manipulate crystal structures. It is part of the Cambridge Structural Database (CSD).

From Mercury's site, it allows you to:

- Generate packing diagrams, define and visualize Miller planes, and take slices through a crystal in any

direction.
- Build and explore networks of intermolecular contacts to gain an understanding of the strengths and weaknesses of structures and identify the key interactions that drive crystal packing.
- Display space-group symmetry elements
- Calculate and display voids (free space in crystal structures) based either on contact surface or solvent accessible surface
- Perform molecule-based gas phase calculations via an interface to MOPAC
- Calculate intermolecular potentials and display e.g. the strongest user-defined interactions in the crystal structure
- View Bravais, Friedel, Donnay and Harker (BFDH) theoretical crystal morphologies.

## 11. IQmol

From IQmol's website:

> IQmol is a free open-source molecular editor and visualization package. It offers a range of features including a molecular editor, surface generation (orbitals and densities) and animations (vibrational modes and reaction pathways).
>
> IQmol is written using the Qt libraries which enables it to run on a range of platforms including OS X, Windows and Linux.
>
> It has been integrated with the Q-Chem quantum chemistry package and offers an intuitive enviroment to set up, run, and analyse Q-Chem calculations. However, it can also read and display a variety of file formats, including the widely available formatted checkpoint file.

It also has a nice user-guide, as well as a YouTube channel. The source code is available on GitHub.

## 12. MOLDEN

Molden is a software tool that allows the display of molecular density from various Ab Initio and Semi-Empirical packages. This tool is capable of reading all the necessary information from the output files of GAMESS, GAUSSIAN, Mopac/Ampac, and several other programs in the Molden format.

Molden offers several features such as the display of molecular orbitals, electron density, and molecular minus atomic density. It also supports contour plots, 3D grid plots, and a combination of both, with the option to subtract either the spherically averaged atomic density or the oriented ground state atomic density for standard basis sets.

In addition, Molden can write graphics instructions such as postscript, XWindows, VRML, povray, OpenGL, tekronix4014, hpgl, hp2392, and Figure. It can import and display several file formats such as chemx, PDB, mopac/ampac, and many others. Molden also has the capability to animate reaction paths and molecular vibrations.

Moreover, Molden allows the calculation and display of true or Multipole Derived Electrostatic Potential and fitting atomic charges to the Electrostatic Potential calculated on a Connolly surface. The tool features an Ambfor standalone force field program capable of optimizing geometries with combined Amber and GAFF force fields.

Furthermore, Molden has a powerful Z-matrix editor that provides full control over the geometry and allows the creation of molecules from scratch, including polypeptides. It was also submitted to the QCPE (Quantum Chemistry

Program Exchange) but its Xwindows version is not up-to-date.

In summary, Molden is an all-in-one software tool that provides numerous features for the display and analysis of molecular structures, making it an essential tool for researchers and scientists working in the field of computational chemistry.

## 13. AVOGADRO2

Avogadro2 is a powerful chemical editor and visualization application that also includes a set of reusable software libraries written in C++. With its updated and improved rendering capabilities, Avogadro2 can handle larger chemical structures and simulations produced by computational chemistry codes. It also supports the visualization capabilities of VTK, making complex visualization techniques possible, such as volume rendering and streamlines. Moreover, Avogadro2 is easy to extend using simple Python scripts and provides access to full-blown C++ plugin APIs where more control is required. Overall, Avogadro2 is a flexible and robust solution for tackling molecular simulation and visualization challenges in key areas of materials science, chemistry, and biology.

## 14. CYLVIEW20 (formerly CYLVIEW)

CYLview is a powerful tool designed to facilitate the analysis and communication of scientific results, particularly for computational chemists. It was specifically created to accelerate the evaluation and analysis of structures, while generating high-quality representations containing all the necessary information for professional publications and presentations. Unlike other programs that have similar functionalities, CYLview was designed to be easy to use and optimized for non-theoretical experimental chemists.

One of the major challenges in preparing publication-quality representations of structures is the need to use multiple programs to achieve the desired result. CYLview overcomes this issue by using powerful visual cues such as fog and focal blur to enhance the perception of depth and direct the viewer’s attention to the desired portion of the structure. CYLview also provides a wide range of visual styles and numerous bond styles to represent various molecular states. It can even reproduce the Houkmol style, which has been used internally in the Houk group for the past 15 years.

CYLview offers an animation module, which allows the creation of movies that smoothly animates the transition between various orientations of the structure. Measurement labels and distance labels can be added automatically, and the precision of the measurement labels can be changed easily. CYLview also includes a function to rapidly generate Newman projections, which are of utmost importance in the depiction and comparison of structures.

CYLview provides a key aspect of the analysis of computed structures, which is the rapid assessment of the number, nature, and magnitude of the various interactions throughout the molecule. The vdW module allows for the examination of steric contacts and the strength threshold of the contacts. The threshold can be changed dynamically to rapidly evaluate the magnitude of the contacts. CYLview also allows for the rapid evaluation of geometry optimizations and frequency jobs from Gaussian 03 and Gaussian 09 calculations.

In summary, CYLview is a powerful tool that offers a wide range of visual styles and functionalities to accelerate the evaluation and analysis of structures while generating high-quality representations containing all the necessary information for professional publications and presentations. Its user-friendly interface and powerful visual cues make it an ideal tool for non-theoretical experimental chemists who wish to use computational chemistry as a practical tool.

## 15. IBOVIEW

IboView is a tool for analyzing molecular electronic structure based on Intrinsic Atomic Orbitals (IAOs). It’s designed to make the complex and often confusing world of electronic structure analysis more intuitive and user-friendly.

One of the key features of IboView is its ability to visualize electronic structure from first-principles DFT in terms of concepts that are easy to understand. This includes things like partial charges, bond orders, and bond orbitals. Even in systems with complex or unusual bonding, IboView can help you make sense of the electronic structure.

IboView is also incredibly fast, and it produces high-quality graphics that are suitable for publication. The program has a simple user interface that is easy to use, even if you're not an expert in electronic structure analysis.

Another great feature of IboView is its ability to import wave functions from other programs like Molpro, Orca, Molcas, and Turbomole. And if you don't have access to these programs, IboView can compute simple Kohn-Sham wave functions on its own using the embedded MicroScf program. You can also use IboView as a plain orbital viewer if you don't need advanced analysis features.

One of the most exciting things about IboView is its ability to visualize electronic structure changes along reaction paths. This is made possible using techniques described in "Electron flow in reaction mechanisms" which can be determined directly from first principles. With IboView, you can explore curly arrow reaction mechanisms and gain a deeper understanding of how molecules react and change.

IboView was developed by the Gerald Knizia group, initially at Universität Stuttgart and now at the Pennsylvania State University. If you're looking for a powerful tool for electronic structure analysis, then IboView is definitely worth checking out.

*This was not an exhaustive list of the visualization applications available for free. These are just some of the applications, I am familiar with.*

*In case, I missed any of your favorites then please let me know in the comments down below to make this list more complete and useful.*

# References:


- What are the freely available crystal-structure visualization softwares? – Matter Modeling Stack Exchange



## 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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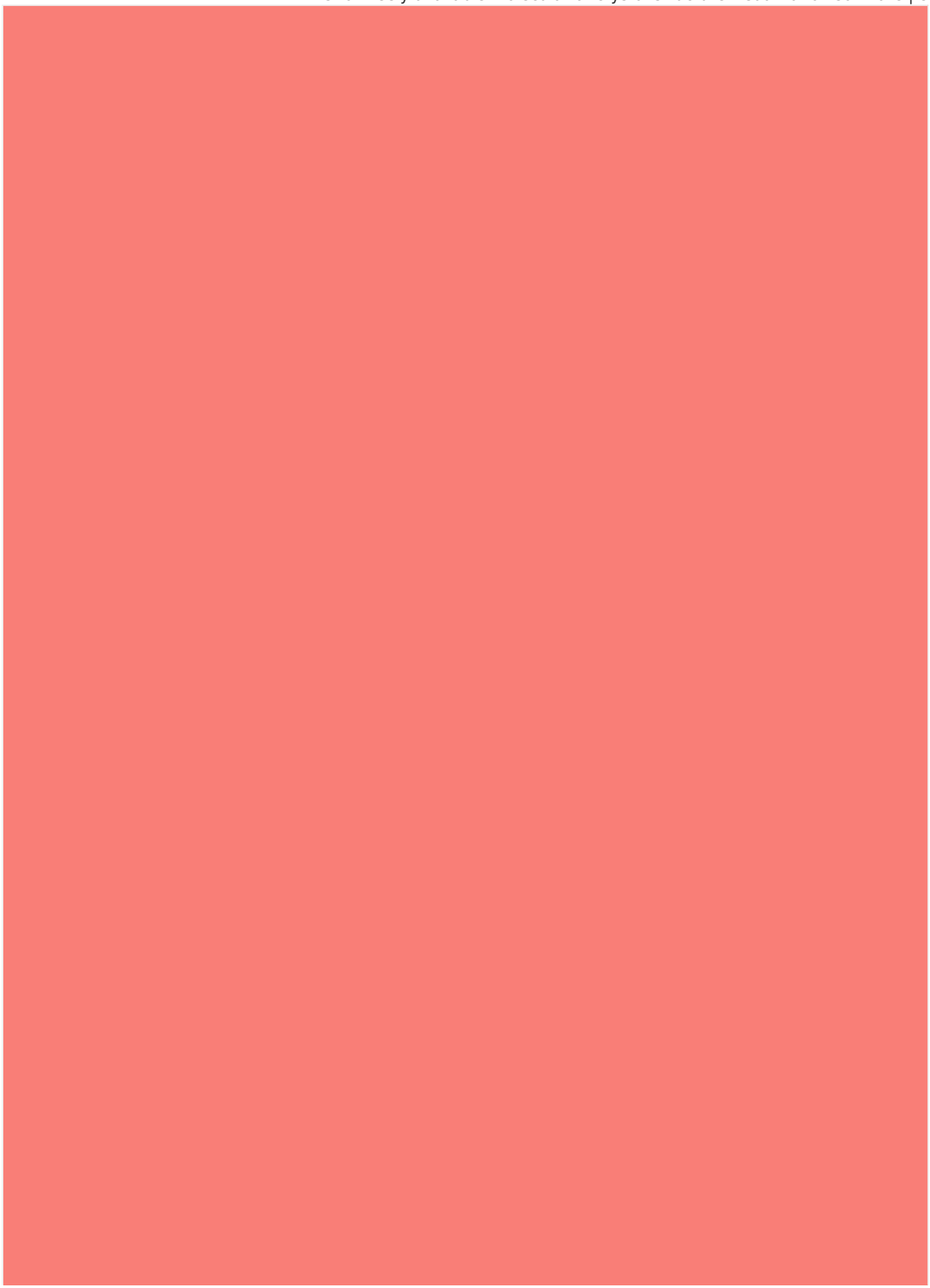

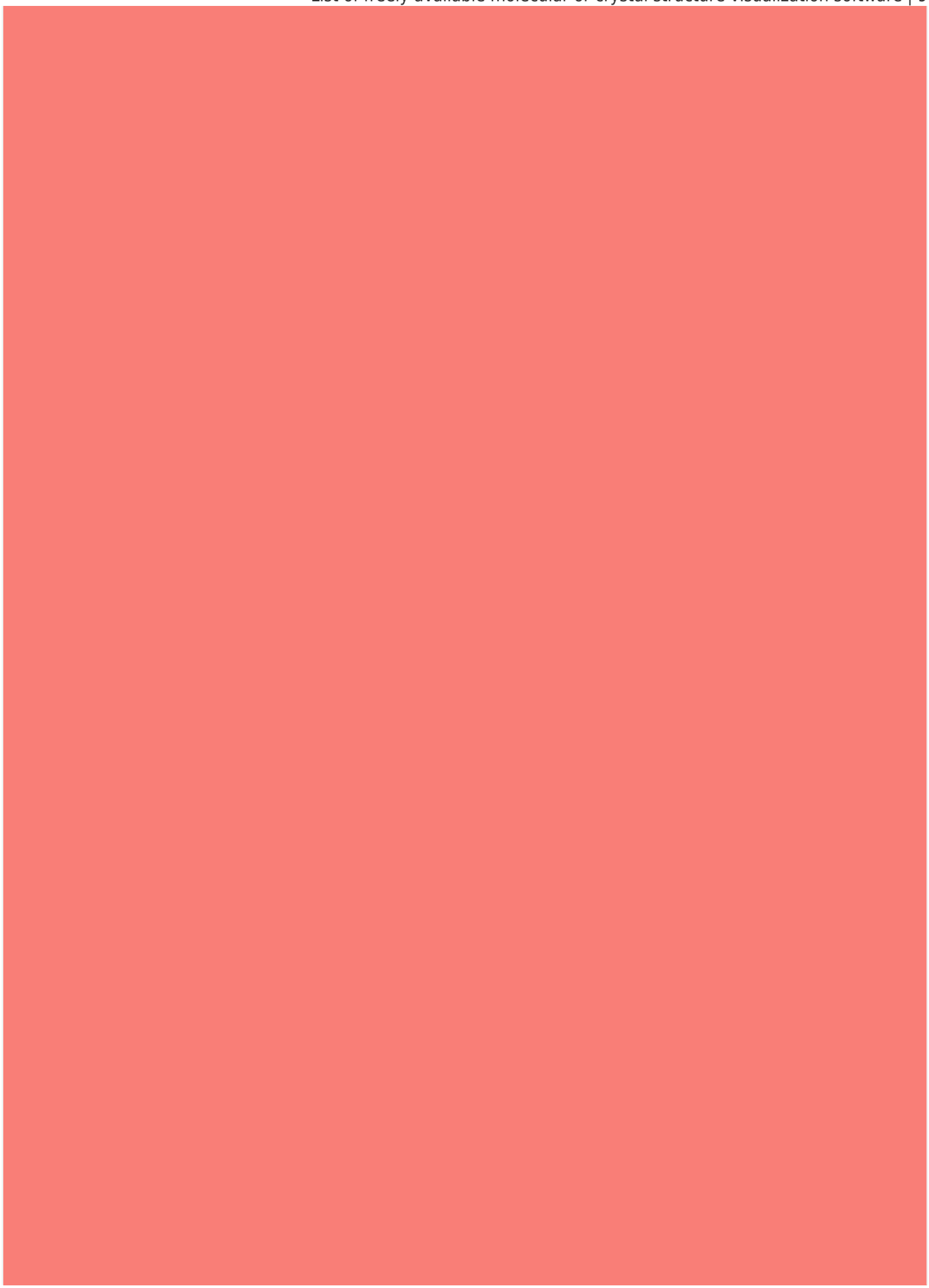

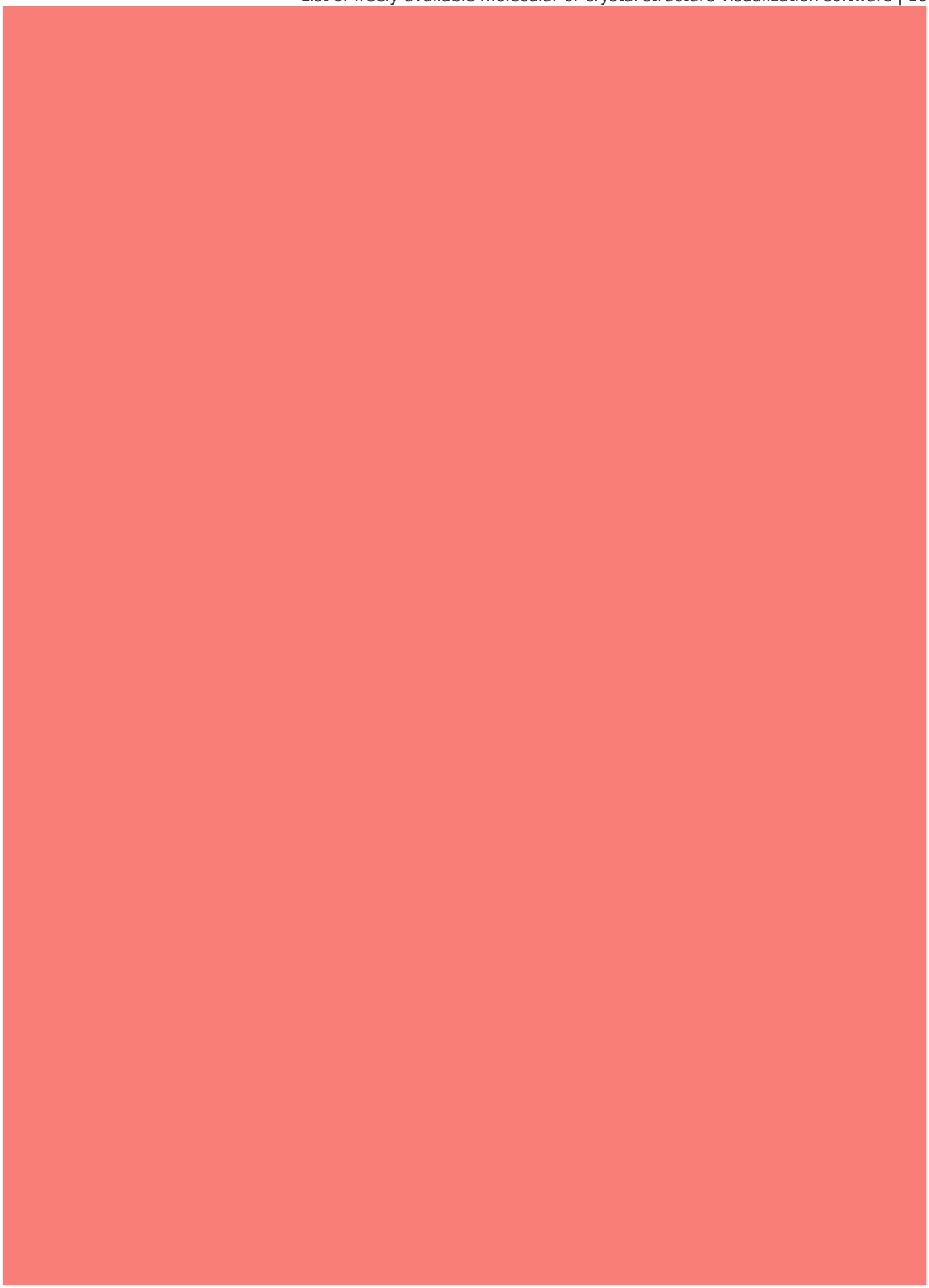

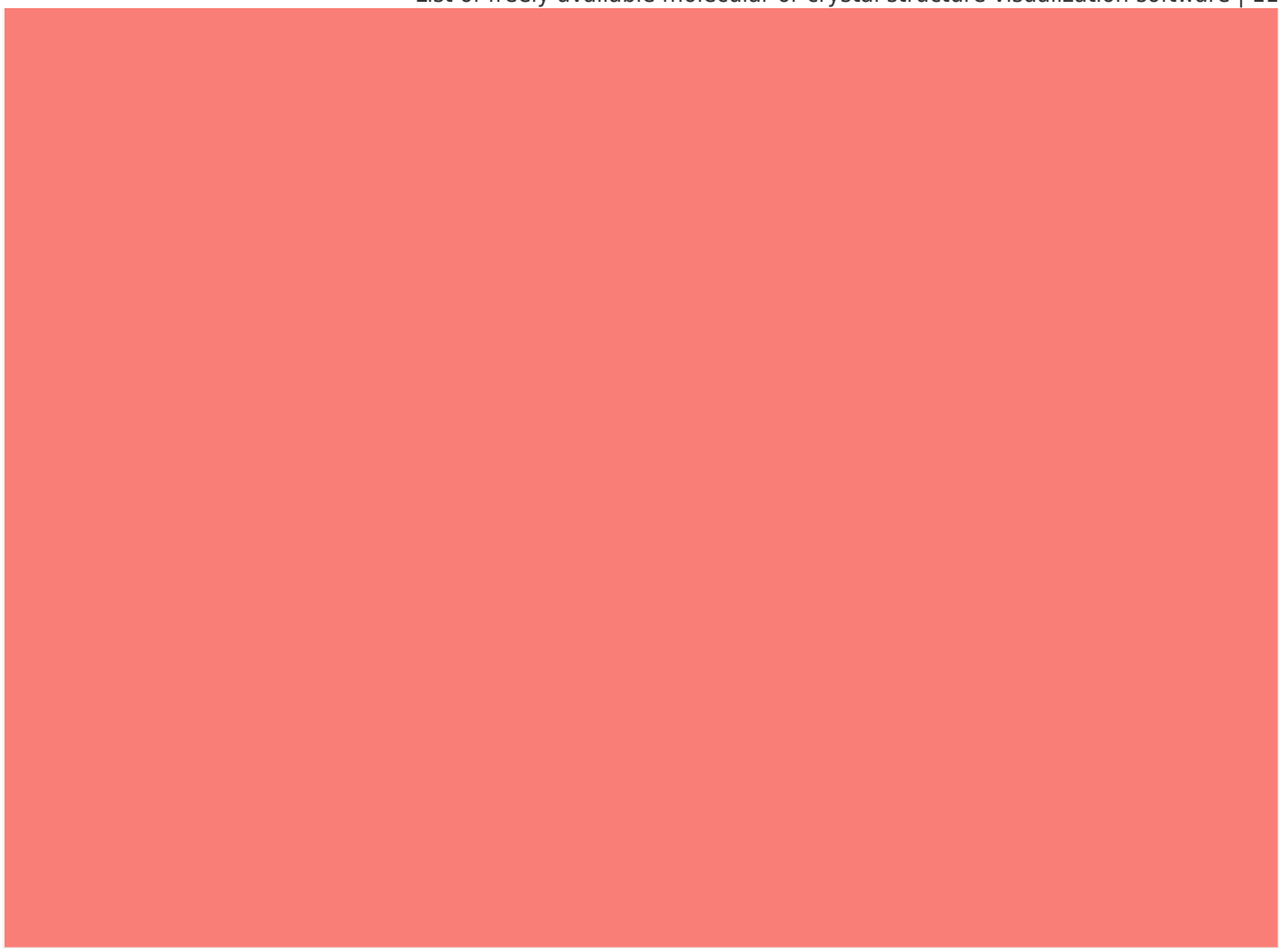

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