

Visualizing Isosurfaces of Electron Density

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INTRODUCTION

- In quantum mechanics, **electron density** or **electronic density** is the measure of the probability of an electron being present at an infinitesimal element of space surrounding any given point.
- In molecules, regions of large electron density are usually found around the atom, and its bonds.
- Electron densities are often rendered in terms of an isosurface (an isodensity surface) with the size and shape of the surface determined by the value of the density chosen, or in terms of a percentage of total electrons enclosed.
- This study focuses on visualizing isosurfaces of electron density around molecules by rendering colorful images and videos using Blender.

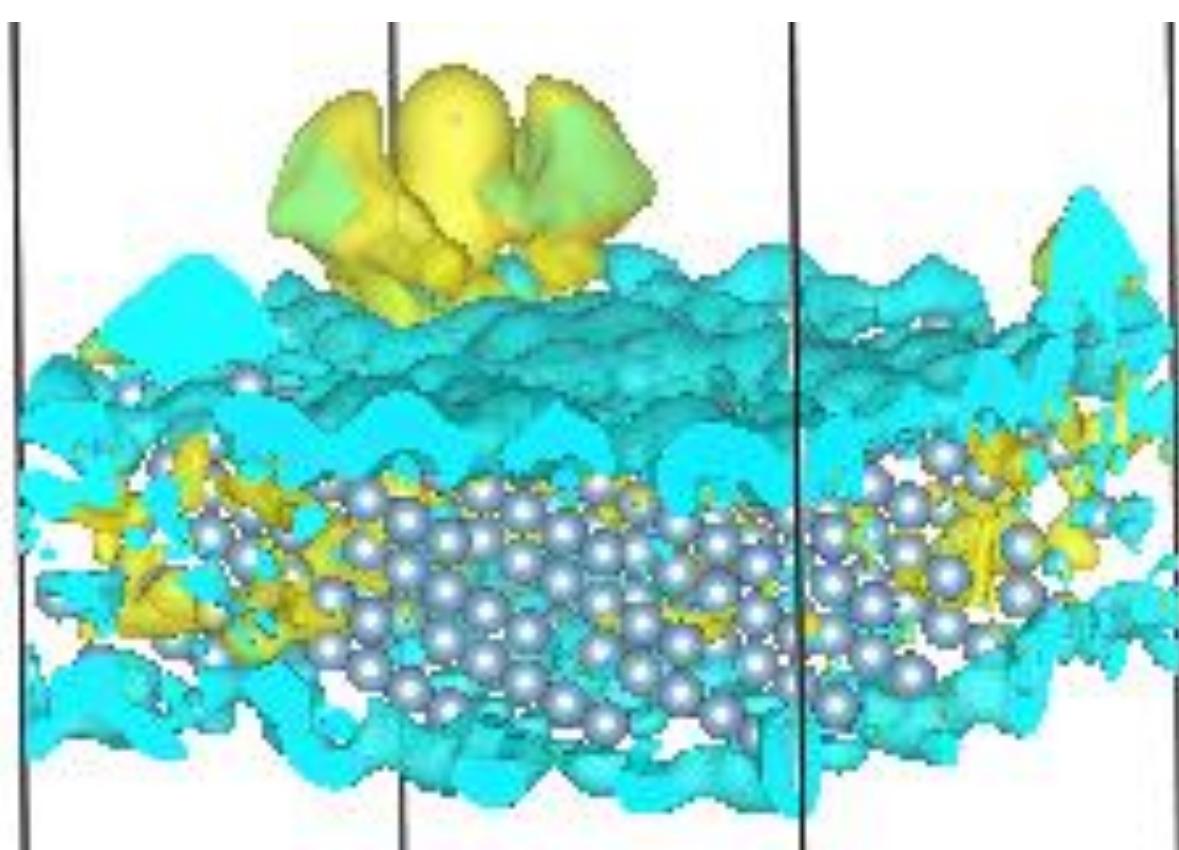


Figure 1: Visualization of isosurfaces of electron density of proton-irradiated Aluminum from the Vesta code.

METHODS

Smoke Simulation

- Blender has a Quick Smoke operator which will automatically create a domain object with a basic smoke material.
- Resolution division of a smoke domain controls the number of subdivisions in the domain. Higher numbers of subdivisions are one way of creating higher resolution smoke, whose data take longer time to compute.
- When enabling Adaptive Domain, the smoke will adaptively shrink, saving computation time by leaving voxels without smoke out of the simulation.

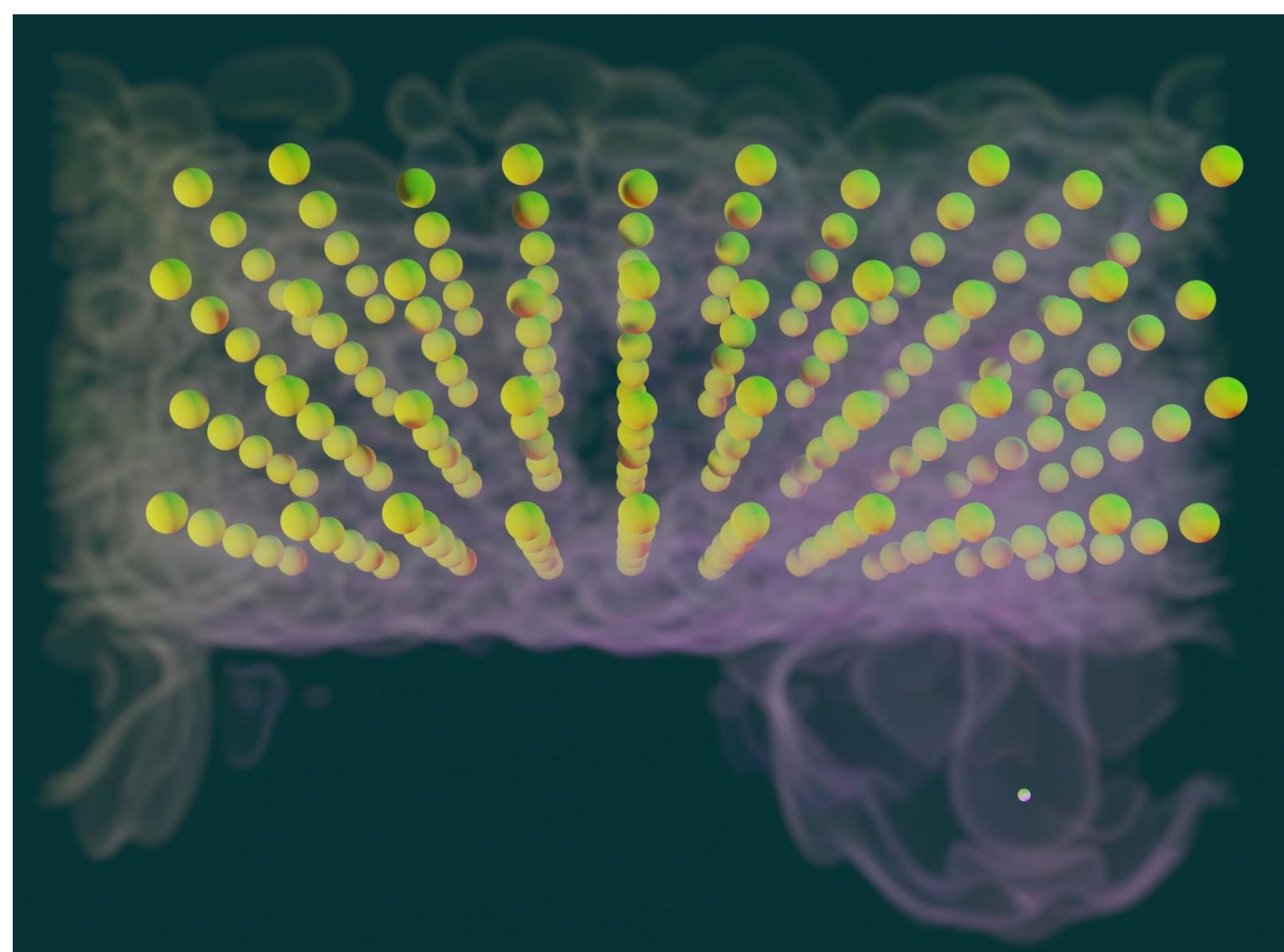


Figure 2: Side view of electron density of proton-irradiated Aluminum

TOOLS

VESTA

- Visualization for Electronic Structural Analysis is a 3D visualization program for structural models, volumetric data and crystal morphologies.
- VESTA can open, edit, and export files that contain electron density data.

Blender

- Blender is a free and open-source 3D computer graphics software that can be used for modeling, animating, creating special effects, and ray tracing, etc.
- Blender can import VRML (Virtual Reality Modeling Language) files that contain data of isosurfaces of electron density that are exported by VESTA.

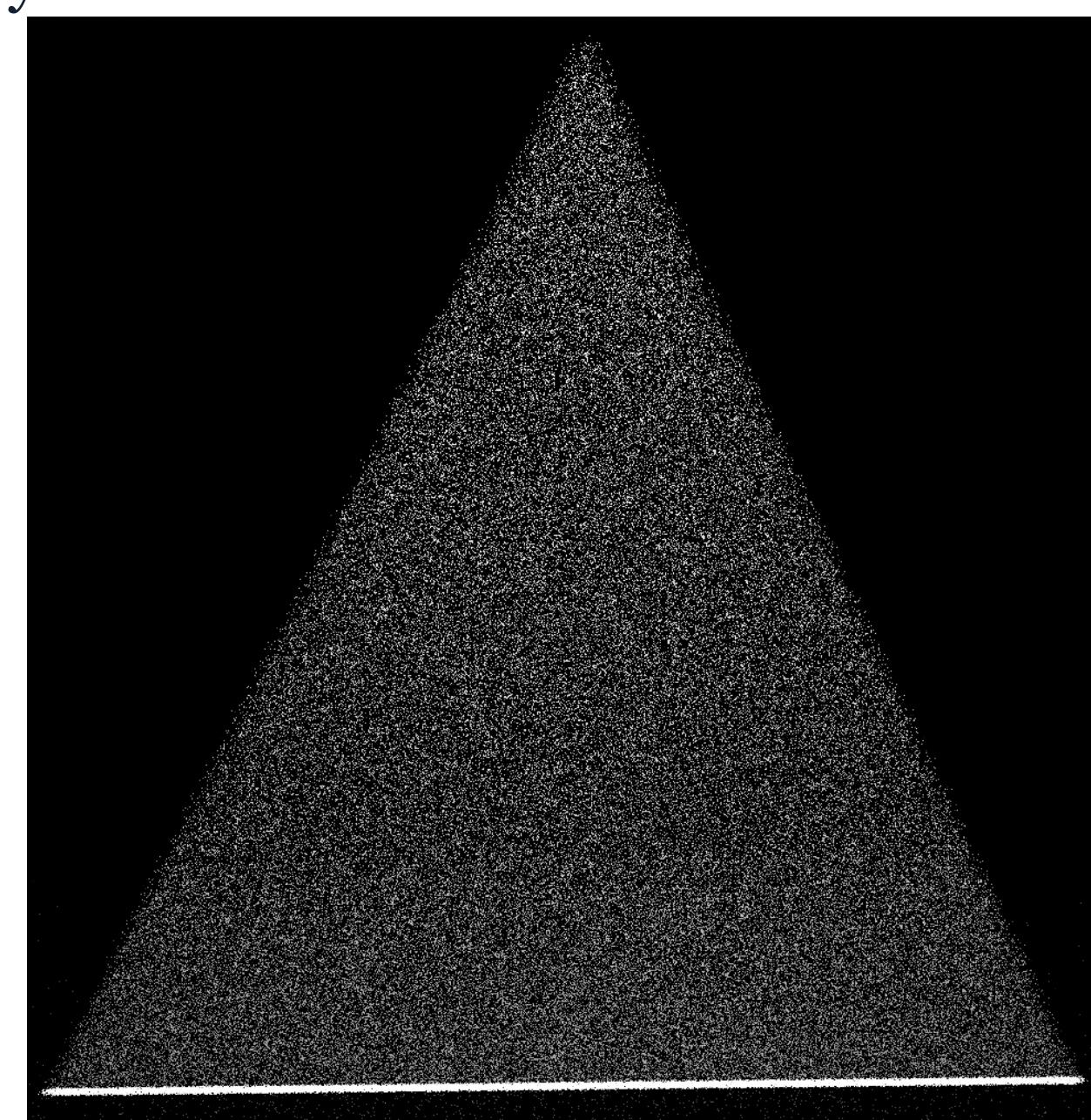


Figure 3: Using image with a white line in node tree of the light source produces a laser plane in Cycles.

RESULTS

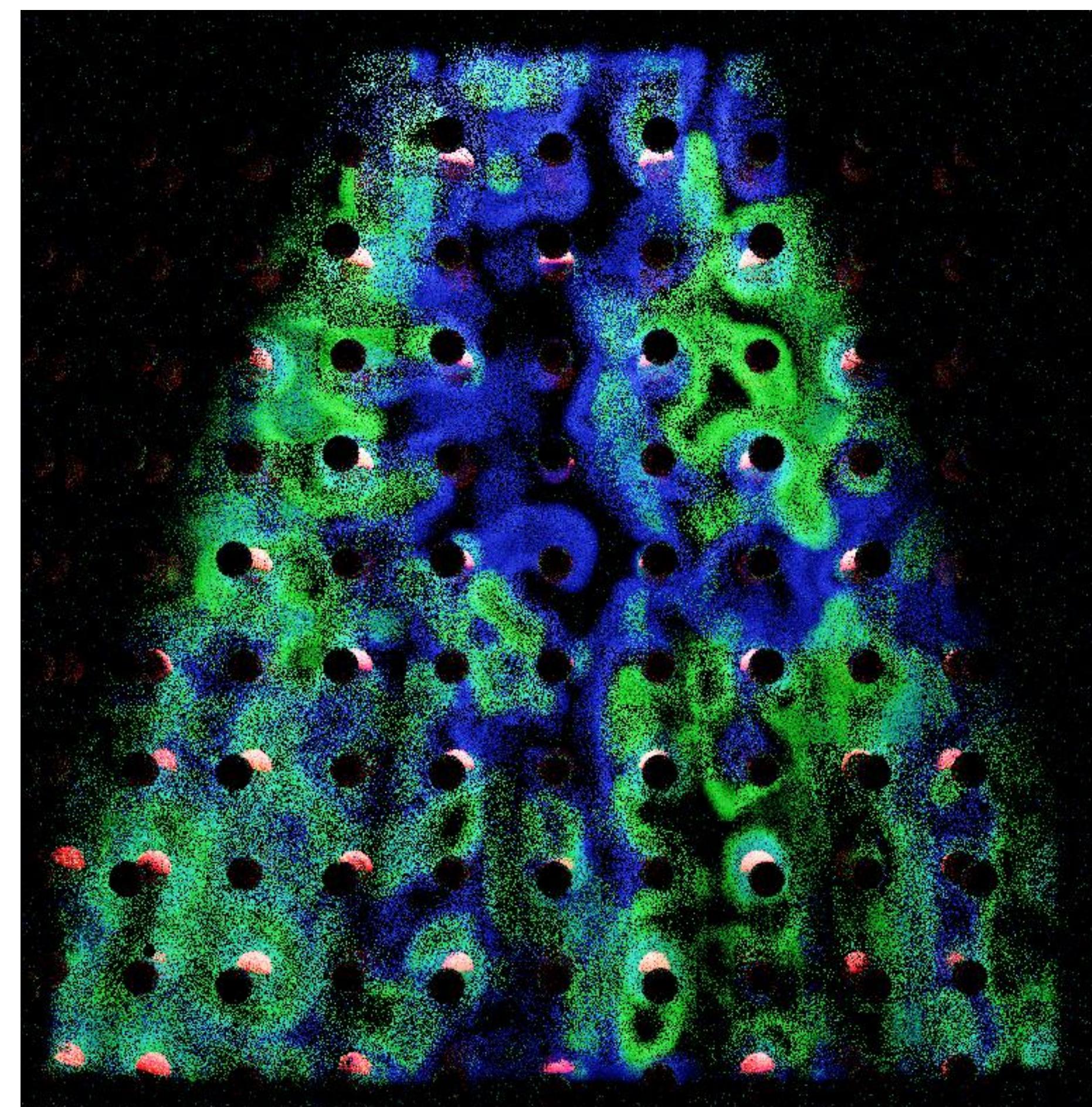


Figure 4: Visualizing cross section of two isosurfaces of different electron density levels with laser plane effect.

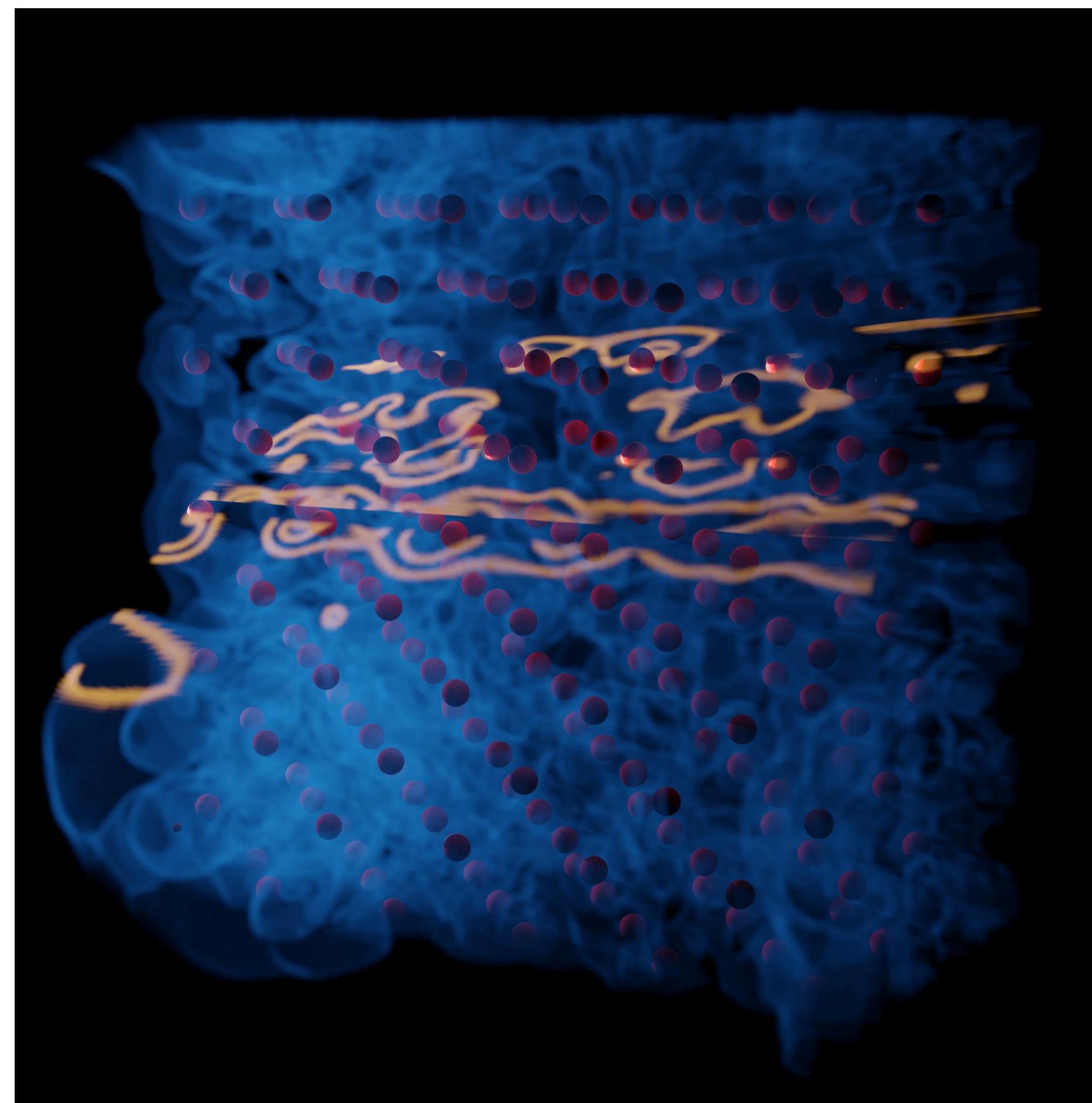


Figure 5: A snapshot of electron density that is ejected from a thin piece of aluminum after an energetic proton impacted the material. These processes happen in radiation environments, including nuclear reactors and outer space, but are also used in research labs to manipulate and characterize materials. From visualizations like this, we learn how the radiation affects the material and the time scales following ion impact.

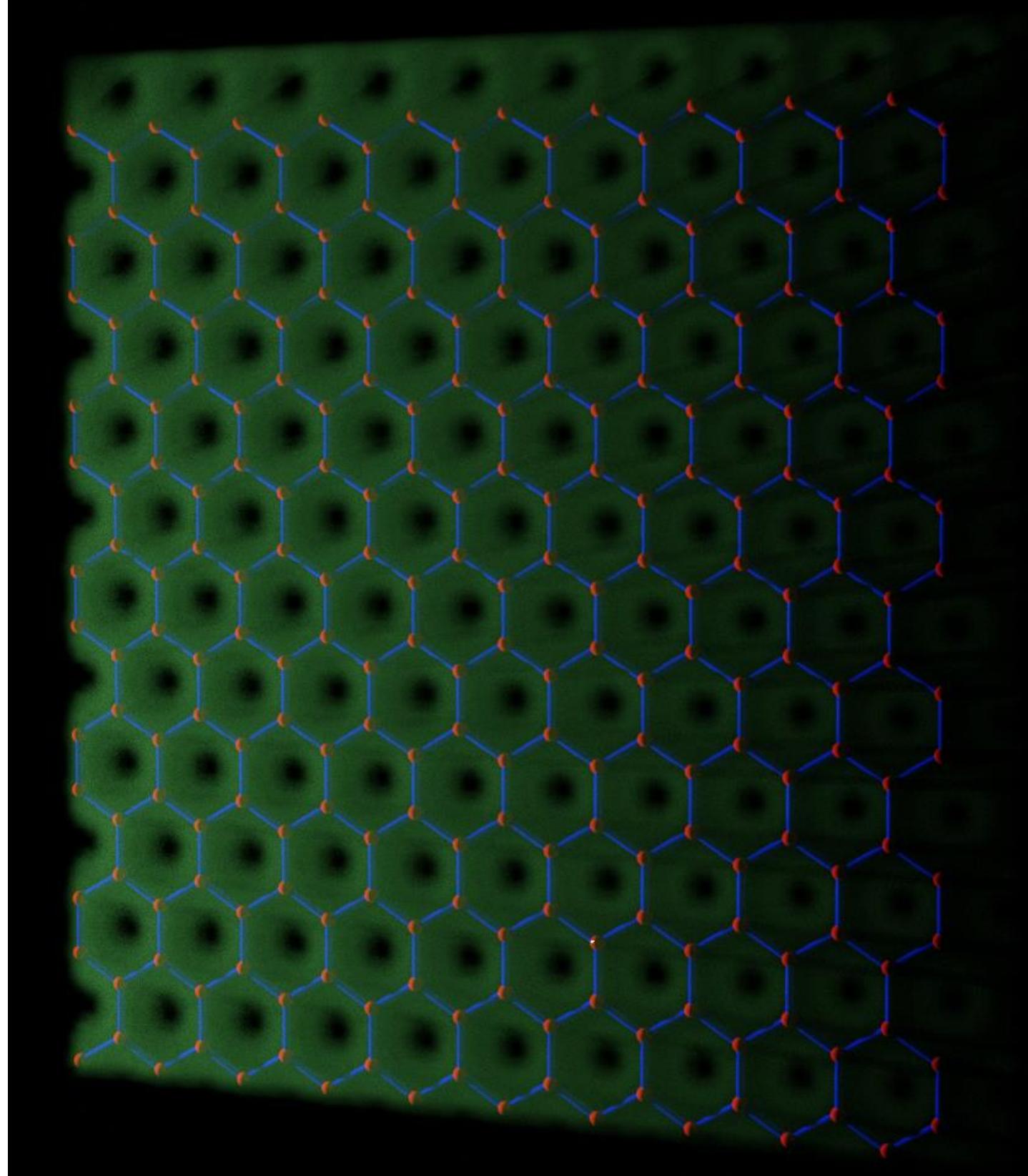


Figure 6: Visualizing electron density, atoms, and bonds of graphene.

CHALLENGES

- Data that contains the shape of electron density should be hidden instead of deleted, because without it the smoke domain cannot rebake the volume data.
- Light color cannot be controlled by the color of the input image, which only affects the shape of light.

CONCLUSIONS

- Blender is a powerful software that can be used to visualize atoms, molecules, electron density, and more.
- Visualizing isosurfaces of electron density in images and videos can help people understand them in a more straightforward way.
- Won second place at 2021 Undergraduate Image of Research competition in UIUC.

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