Visualization of Electron Densities of Gold Atoms Using XCrySDen Program

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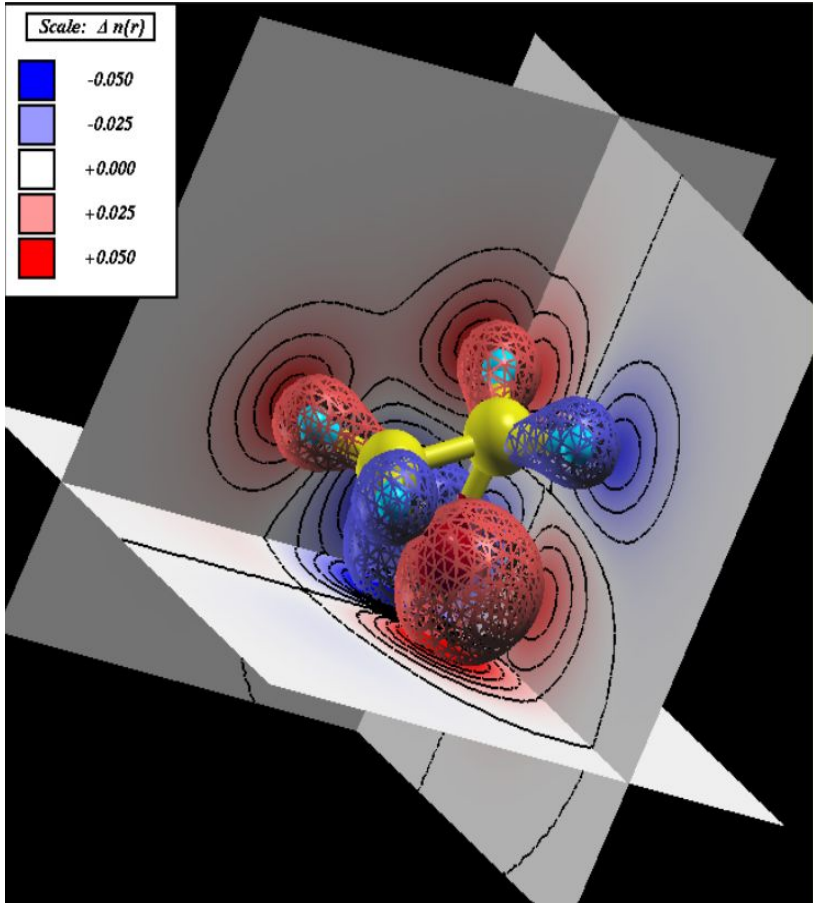
General Idea of the Project

- **XCrySDen**: Crystalline and molecular structure visualisation program

What can this Program do?

- Output isosurfaces and contours
- Rotate the display and move the planes



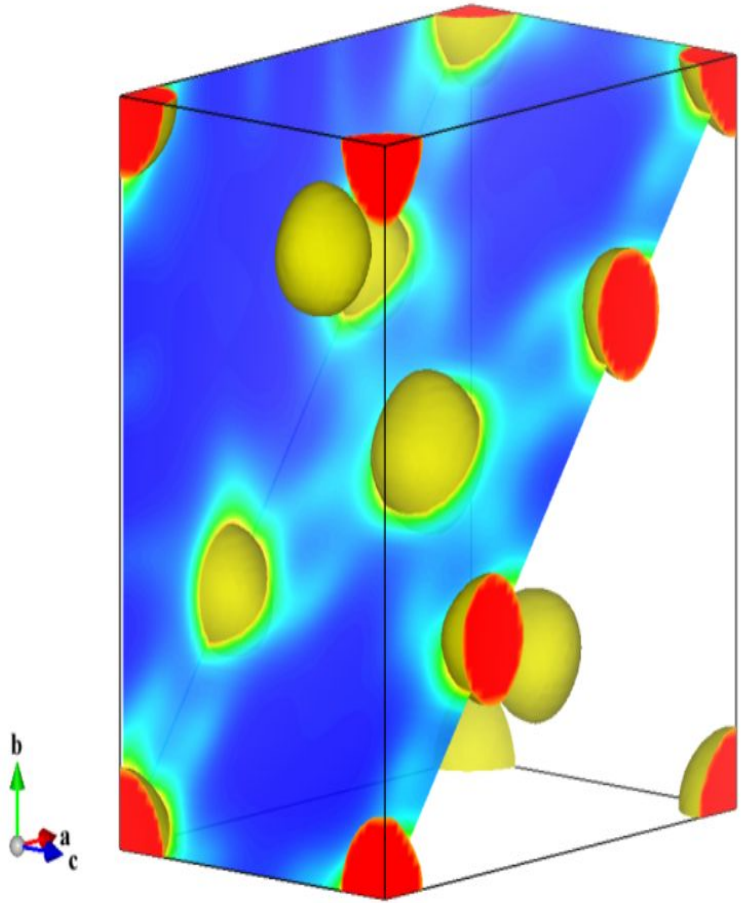
HOMO (Highest Occupied Molecular Orbital) of oxirane →

Purpose

- Is this program useful for Dr. Bumm's research?
- Electron densities: probability of finding electrons in a specific location
    - From isosurface planes and contours
- There is not a clear problem for research
    - Study the plots

Goals

- Plot the electron densities of the gold atoms
- WAVECAR file data:
  - Number of bands
  - Energy levels
  - Wavefunction
- Combinations of the crystalline structures
- **VESTA:** 3D visualization program for structural models and volumetric data



Any Questions?