

## Visualization of Electronic Density of Nanotube with AViz

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Three-dimensional visualization of charge density is challenging, especially when several molecular/atomic levels are intertwined in space. One approach we explored by a recent project to solve this issue: the extension of an anaglyphic stereo visualization application based on the AViz package for hydrogen atoms and simple molecules to larger structures such as nanotubes. The reason for doing so is that the spatial volume occupied by an atom depends on its electronic density, and this density can only be evaluated exactly for hydrogen-like atoms, but there are many excellent algorithms and packages to calculate it numerically for other materials.

The use of AViz dot-mode visualization for electronic density was first developed in an undergraduate project about the hydrogen atom. We then visualized the electronic density resulting from simulations of larger molecules and solids in the same way.

The next stage in our visualization development was to move to 3D stereo. Stereo Vision (SV) works by showing a different image to each eye, thus creating the illusion of a 3D image. AViz 6.1 incorporated the possibility of SV, and although more than two colors are possible there remains some color washout, depending on color selection. The SV images generated by AViz, are best viewed using red-cyan anaglyphic glasses. Stereo Visualization was applied to the electronic density of the hydrogen atom by Meital Kreif.

We selected the public domain code Quantum Espresso (QE) plane-wave DFT code which has clear documentation of their format for the charge density, in order to measure the width of a nanotube wall, which needs the calculation of the electronic density. For this calculation We chose the vdW-DF non-local correlation functional with the C09 exchange functional in order to account for London dispersion interactions (or van der Waals forces) within our calculations. We found that color binning and some random dilution optimizes the possibility of “transparency” into the samples.