



Mini-review of Electron Density Visualization

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Abstract

We describe both educational and research oriented examples of electronic density visualization with AViz. Several detailed cases are presented and the procedures for their preparation are described.

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1. Introduction

The wavelike nature of atoms, molecules and solids is a difficult concept for students to grasp. Since Rutherford we have known that atomic nuclei only take up a small part of atomic volumes, however the nuclei do not approach each other too closely because of the electronic density surrounding them. Electronic wavefunctions are known analytically for hydrogen and hydrogen-like atoms; but for other atoms and all molecules and multi-atom materials a numerical approach is needed.

There are many cases where the nature of the electronic wavefunctions needs to be understood. The first of these occurs in undergraduate quantum mechanics courses. Writing a complicated wavefunction including spherical harmonics does not immediately help students gain insight into atomic symmetry. When they are struggling with the particle-wave duality of atoms, orbital shapes can help gain insight. Explanation of different forms of inter-atomic bonding, with the canonical example being the structure of carbon allotropes wherein sp^2 and sp^3 wavefunctions give different geometric lattices, is much easier if the spatial nature can be shown.

Many materials require comprehension of their electronic density to understand their structures. Nanotubes are the classic example, where the width of the nanotube wall has to be deduced in order to model, for example, vibrational behaviour. Bending and stretching properties are important and the bending of the tube is limited by the wall width.

2. Visualization

Electronic density is three dimensional, and varies in density as functions of distance from the nucleus and of angle. Two dimensional cuts and even successive slices are not always helpful except for very simple uniform cylindrical cases. Visualization techniques such as rotation, zoom, and building up images layer-by-layer are helpful. Partial transparency also gives insight. Stereo vision is good; and stereo with limited cost can be important for educational use. All these techniques can be implemented in the public domain AViz (Atomistic Visualization) package [1, 2], developed at the Technion and now part of the FP7 SimPhoNy project [3].

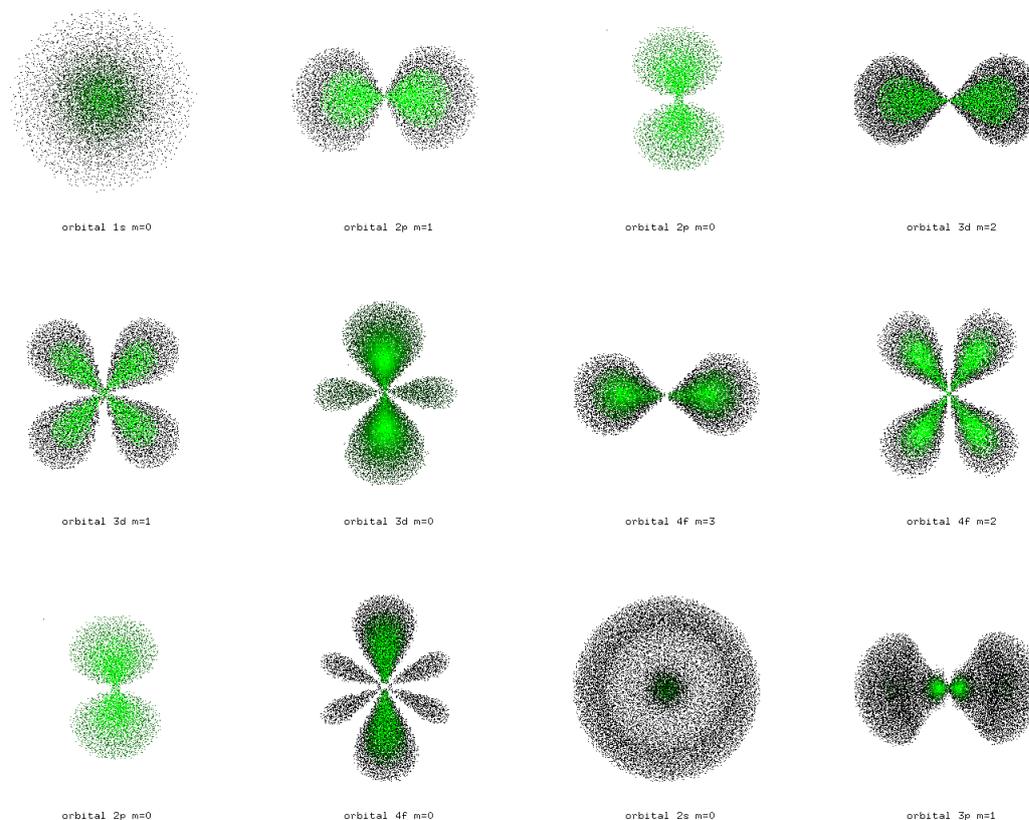


Figure 1. AViz dot visualizations of electronic density of states of an H atom.

3. The educational hydrogen atom case

When students first meet hydrogen atom wavefunctions they often have difficulty grasping that s orbitals are symmetric in radius, r and angular states, p, d, f are not. 2D graphs cannot not show this. A beautiful old figure (1930s) of White [4] shows hydrogen atom wave functions, pictured by photographing spinning tops. The smoke rendering visualization technique can be used to show electronic density but this is usually done with white “smoke” [5]. When we were developing the AViz visualization package for atomistic simulation and discussing how to show electronic density we thought that perhaps, applying it off-label using the dot representation would work. We found that using an extensive color palette was very confusing, but binned color worked quite well.

The initial procedure was quite straightforward, as developed by Joey Fox [6, 7]:

- Use MATHEMATICA to express the analytical solutions for hydrogen atom wavefunctions, which are in spherical coordinates at a mesh of cartesian points.
- Calculate the x, y and z coordinates of points in the volume element around each point, whose number (and color) correspond to the electronic density at the central point.
- Prepare $.xyz$ files in the AViz format - one line with number of points, followed by a comment line, followed with a line for each point that has type, x, y and z coordinates as real numbers and additional columns containing for example the actual electronic density at that point as real numbers.
- Apply AViz in dot visualization mode using binning of color density.

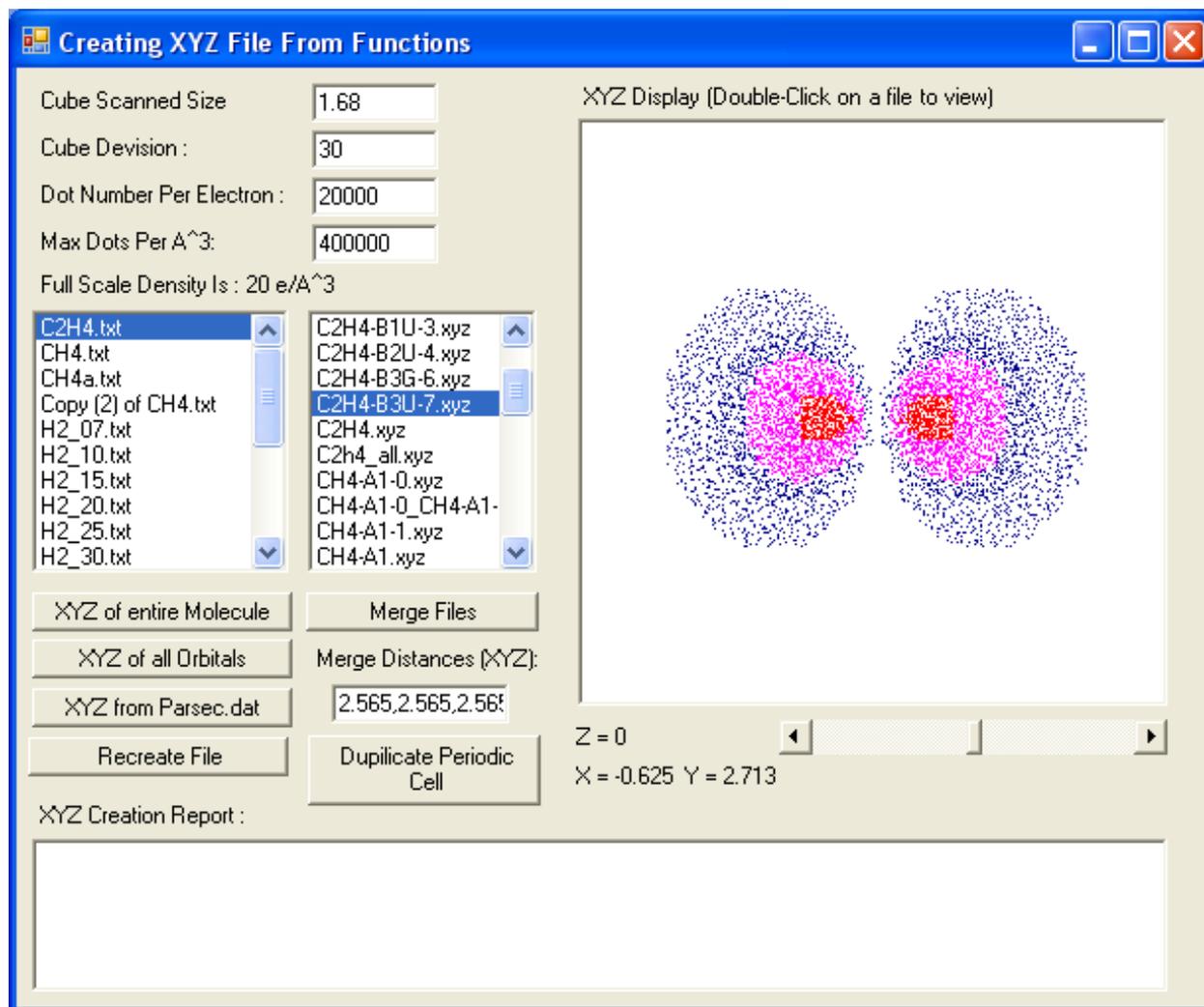


Figure 2. Interface of program to convert PARSEC output into AViz .xyz format.

With a suitable choice of dilution and binning, images that can be rotated or sliced are found.

In order to extend the visualization quality, after analoglyphic stereo was introduced to AViz [8], the hydrogen atom visualizations were extended to stereo by Meital Kreif. The procedure is identical, although the color selection is different so that the AViz stereo option can be turned on. We show a selection in Figure 1; this figure shows exactly the same selection and order as the initial selection of orbitals in [4]. These images, and especially the animated versions accessible on the website [10] enable students to understand the difference between spherically symmetric s states and p states.

4. Beyond the analytic solution cases

We now consider other atoms and simple molecules whose electronic density can be calculated numerically in many different ways. Or Cohen [11, 12] calculated it within Density Functional Theory (DFT) using Slater Type Orbitals (STO-3G) using PCGAMESS or PARSEC. The latter calculates on a grid so the visualization procedure is the same as for the hydrogen atom from then on. Rather than the use of MATHEMATICA, he prepared a code in Microsoft C#.Net that takes the output of e.g. PARSEC and prepares a grid and fills it with dots. In Figure 2 the interface of his code is shown.

Ethylene's Molecular orbitals

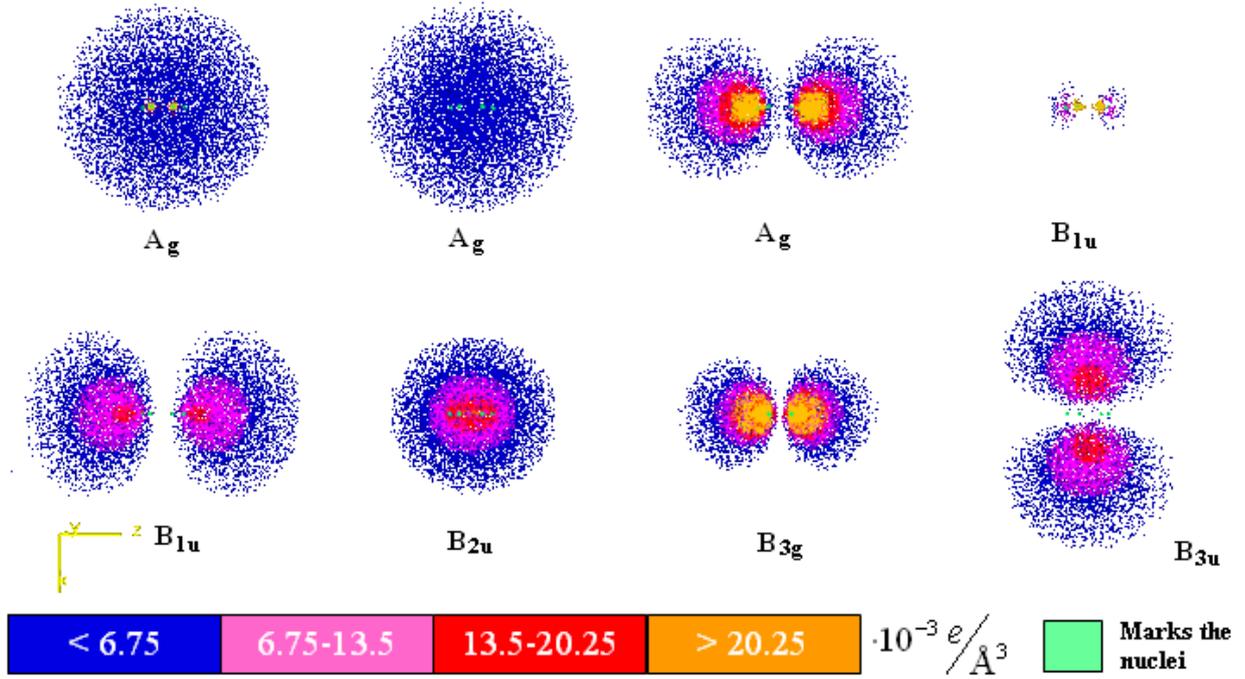


Figure 3. Sliced, separated orthogonal orbitals of ethylene calculated from PCGAMESS, with color legend.

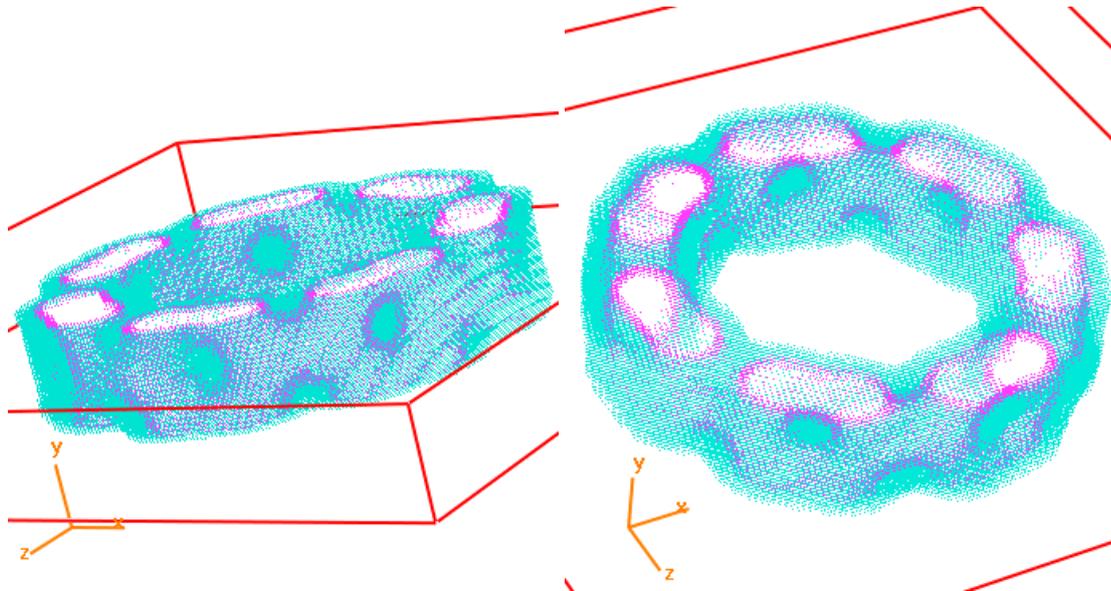


Figure 4. Two diluted images of the electronic density of a single nanotube ring, calculated with QUANTUM ESPRESSO.

The ethylene molecule consists of two carbon atoms which have both π and σ bonds between them, bonded to 4 hydrogen atoms creating a planar structure. This molecule displays the carbon's sp^2 hybridization. A natural ethylene molecule contains 16 electrons. The wavefunction for the electrons were produced by the PCGAMESS programme again using the STO-3G basis set. The electronic densities are calculated as separated orthogonal orbitals, each of which consists of a certain symmetry of the D2h point group. In this case 5 symmetries are used - Ag, B1u, B2u, B3g, B3u. Notice that the distance between the two carbons is 1.317 Angstrom and between each carbon and its closest hydrogen atom is 1.076 Angstrom. The different orbitals are shown in Figure 3.

The results described in this and the preceding section were entirely obtained by undergraduate students in either Computational Physics class or final undergraduate projects.

5. Carbon allotropes including nanotubes

The natural extension of this project was to visualize carbon allotropes, which have been a major focus of the Computational Physics Group at the Technion for a long time. Both diamond/graphite transformations and nanotube transport and modelling applications have been studied. The former led to two AViz enhancements [13], variable bond lengths and change of fovy (fixed angle of viewing in the y direction). The latter is very helpful for avoiding moire effects in the electronic density dot/smoke applications. The first steps in the carbon allotrope direction were made with VASP and VESTA visualization, and have been described in [12]. These results were of the contour map variety, rather than the smoke type, however they validated the results from the previous section, rather nicely.

We were finally able to obtain dot/smoke visualization images for nanotubes with the use of QUANTUM ESPRESSO code. Details and many examples are given in [14] and were presented at CSP2015. We conclude with two different angles of a visualization of a single ring with a color selection enabling good transparency, in Figure 4. This data file can be found at [15] for readers who wish to try out the visualization for themselves.

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