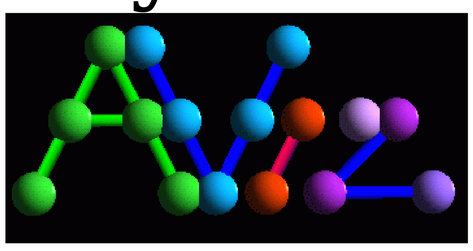
# Visualizing electronic density of atoms and molecules with



Joey Fox, Or Cohen, Eduardo Warszawski and Joan Adler - Technion

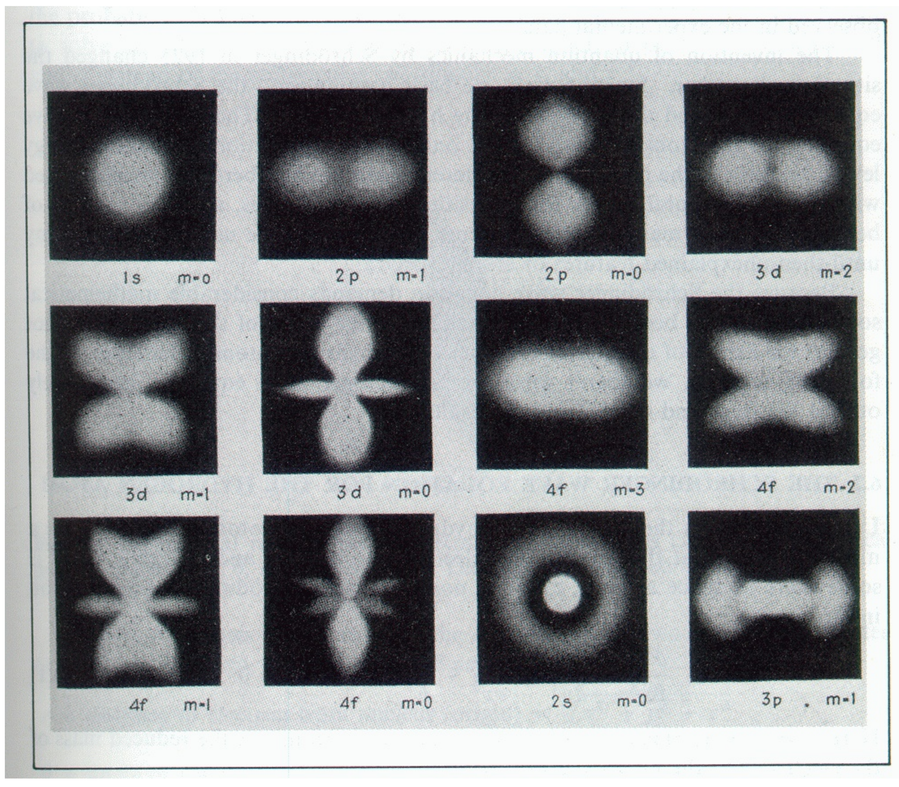
## INTRODUCTION

The three-dimensional nature of the electronic wavefunctions of the hydrogen atom for different states is subtle and almost impossible to comprehend from a two dimensional drawing.

A classic set of photographs of electron clouds (presented by H. E. White in ``Introduction to Atomic Spectra'', 1934) made from spinning wooden models for several energy states of the H atom is reproduced on the right.

72 years later we can do a bit better and using an ``offlabel'' implementation of the AViz atomistic visualization package we have created three-dimensional visualizations showing clearly the geometry of different states.

Dots with densities corresponding to the electronic probablility density and color coding to emphasize more dense regions as well as slicing and rotation to aid depth perception are implemented. In this poster examples of hydrogen atoms and molecules, lithium atoms and ions and methane and ethylene molecules are shown.




## HYDROGEN ATOM - Analytic Solution

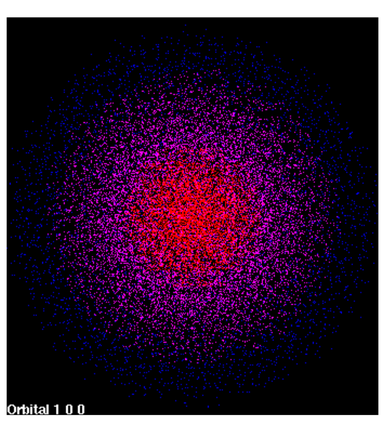
For the hydrogen atom the densities can be calculated from the analytic solution of the Schoedinger Equation. There are three quantum numbers,

*n* is the quantum number arising from quantization of energy

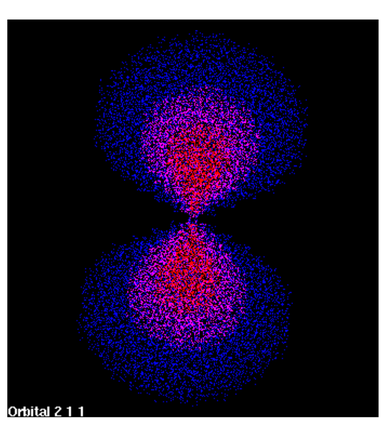
*m* is the quantum number arising from quantization of angular momentum

l is the quantum number arising from quantization of angular momentum squared

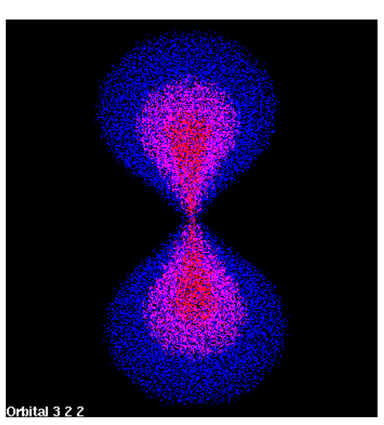
We visualize the probability of finding an electron for a given *n.l.* and *m* below. The colour gradient runs from low density (blue) to high density (red) .



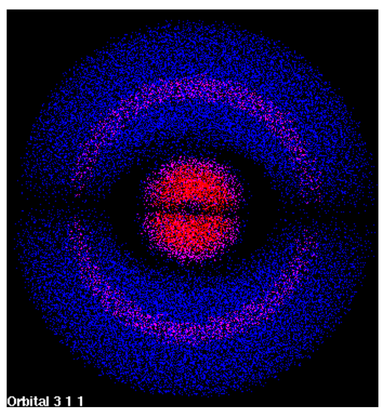

(1,0,0)



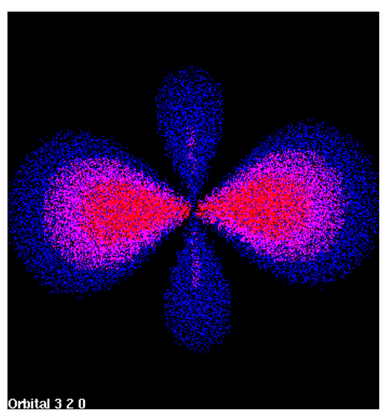

(2,1,1)



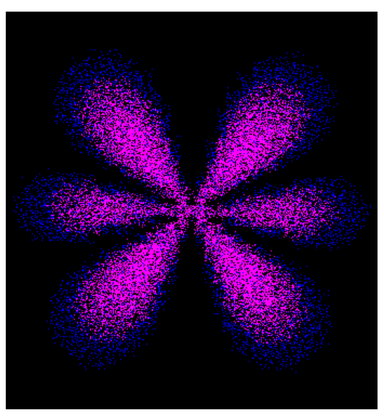

(3, 2, 2)



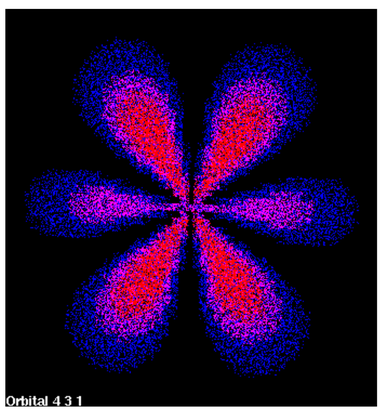

(3,1,1)



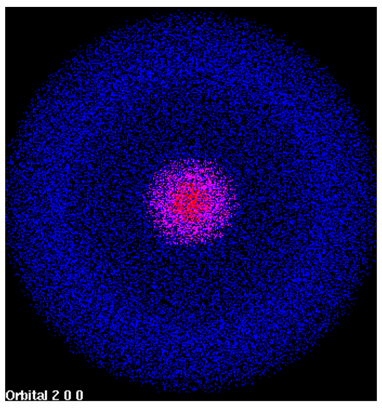

(3,2,0)



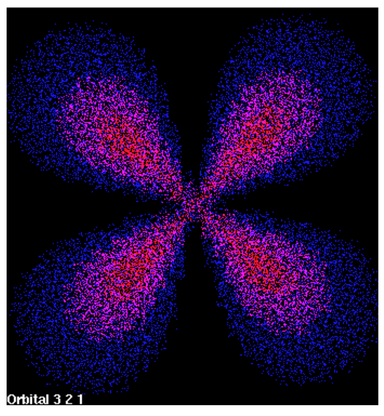
(5,4,2)




(4,3,1)




(2,0,0)




(3,2,1)

The AViz package was created by Geri Wagner and Adham Hashibon, based on earlier OpenGL routines written by David Segev (Saada) and implemented by Irina Rosenblum amongst others.
It takes a .xyz file of atomic coordinates, and draws balls at the atomic sites and then adds bonds on specific lengths between specific atoms, thus enabling us to directly observe bond lengths and angles. The color code implementation is discussed at http://physics.technion.ac.il/~eduardo/aviz/aviz_gradient.html
More details at http://phycomp.technion.ac.il/aviz

## MOLECULES, ATOMS and IONS -

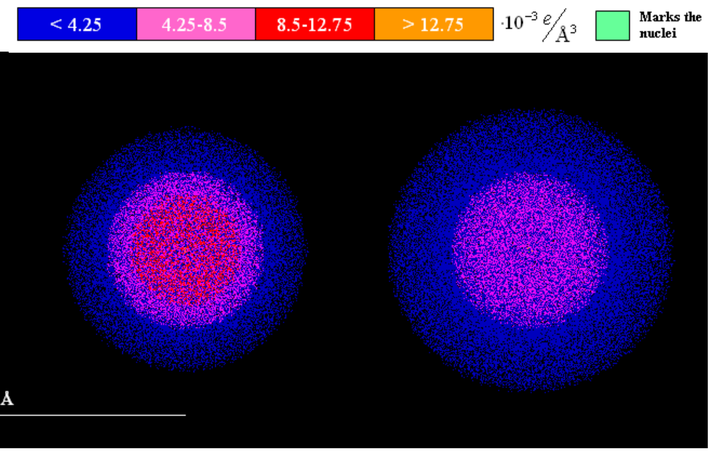
### NUMERICAL SOLUTION with DFT

For other cases numerical solution of the Schroedinger equation is needed, nevertheless, this approach has been extended to more complex systems. Density Functional Theory was applied to lithium atoms as well as to hydrogen, methane and ethylene molecules.

Density functional theory is based on calculating the complete electron density of the ground state of the atom or molecule. The Hamiltonian is defined as a functional of the ground state density, but this density is calculated as an eigenstate of the Hamiltonian. Using iterative calculation the Hamiltonian is varied so that the energy is brought to a minimum in accordance with the variational principle. The color codes differ for each case and are shown alongside.

More details at http://phelafel.technion.ac.il/~orcohen We thank Leeor Kronik for help with the computations.

### Lithium




Left to Right

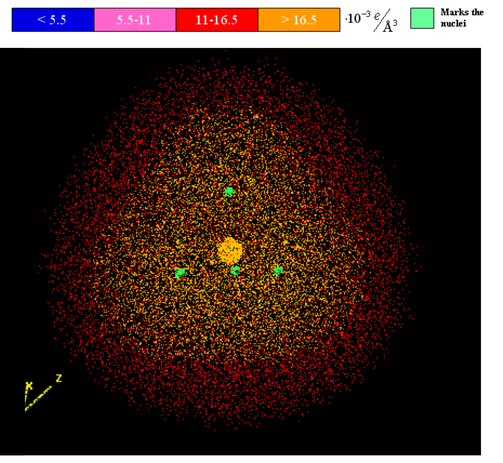
Positive Li ion

Li atom

negative Li ion

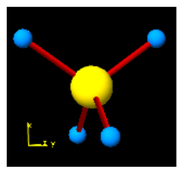
in true size

### Methane

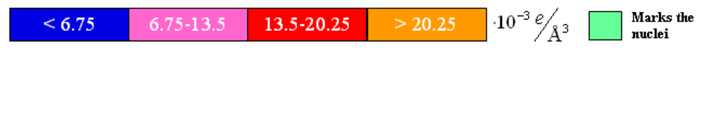



Left - entire molecule

Right - highest density



### Ethylene




Left - entire molecule

Right - sliced thru the middle plane