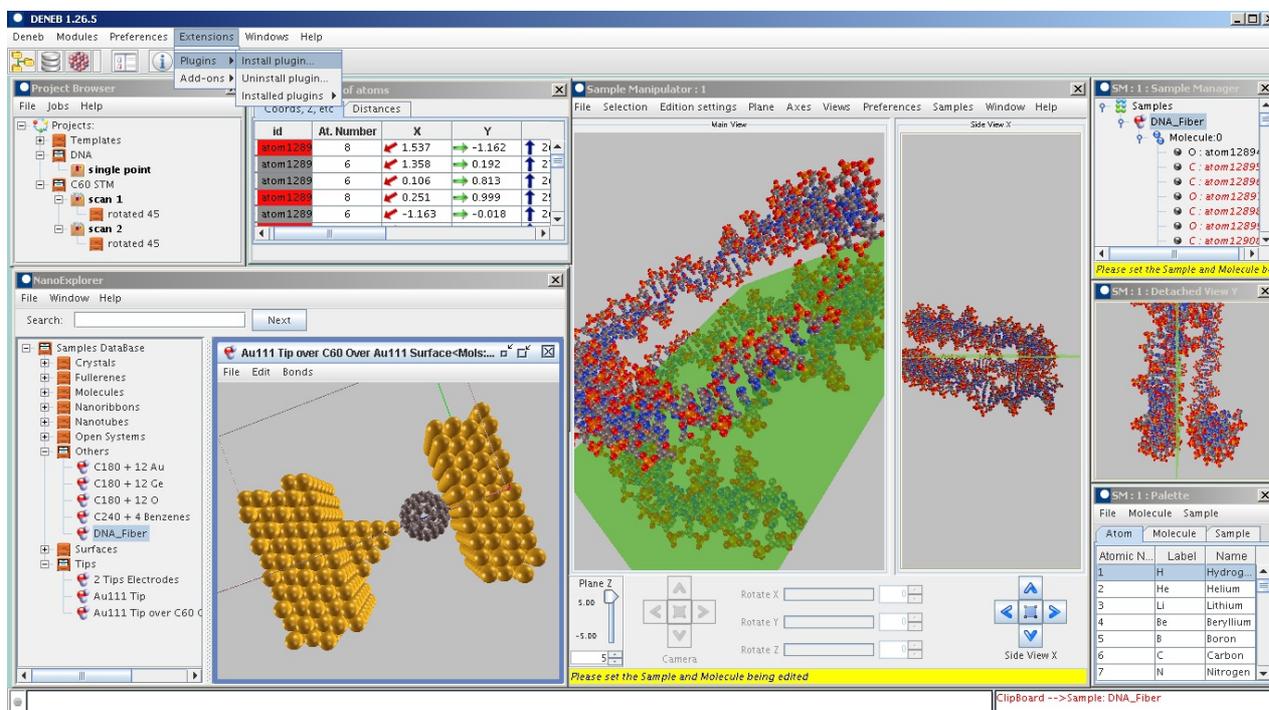


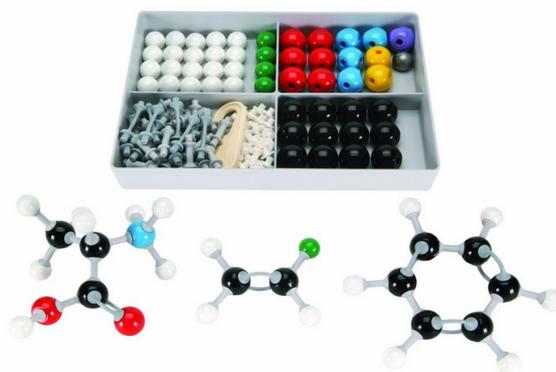
DENEb



id	At. Number	X	Y
atom1289	8	1.537	-1.162
atom1289	6	1.358	0.192
atom1289	6	0.106	0.813
atom1289	8	0.251	0.999
atom1289	6	-1.163	-0.018

Experience The Nanoworld With **Atelgraphics**

Do you remember the molecular modeling kits? It looks like this:



The shiny colorful balls in the box are atoms. When arranged in different geometries, atoms form molecules. For example, see the molecule at the right, it is composed of six C atoms arranged in an hexagon plus six H atoms around it: it is a benzene molecule.

This is a very nice toy to communicate your ideas: --“Look Bob, this is the molecule I am talking about”, and you assemble before Bob the molecule you mean to show.

Nevertheless, it is sometimes not practical, or not quite enough, for several reasons:

- You usually can not carry it with you. So most of the time you can not show your new molecule idea simply because the kit is not at hand.
- You run out of C atoms again! Yes, as soon as you need to make a larger structure, a carbon nanotube for example, you use them all and you are only half way through.
- The links between atoms are sticks at certain angles, but new studies reveal new nano-things where those angles are not necessarily so ... and you want to show that new model.
- The links between atoms are sticks of certain lengths, but you really want to model a nanowire that it is stretched and about to break, this means the distances increase before the breaking point.
- Single plastic sticks or double sticks are ok, but they are crude representations of electron densities ... Yes, you really would like to see what is the real shape of the electron cloud that glues atoms together. What is the shape of the molecular orbitals?

- "I sometimes want to increase the size of some atoms or bonds just to highlight some parts", I would be happy even by being able to change the black color by a dark grey of just some of the C atoms, not all of them (for example)
- Once I have my molecular model defined ... how I wish that it would tell me how chemically stable it is, how hard or elastic it is, what are its vibration frequencies and modes, I wish to see it vibrating at low temperatures, and ... why not, I want to see it breaking when overheated ...

But of course many of these things I can only imagine ...
Or do I?

All the above are easily overcome by **DENEb**, the software that spells modeling freedom and power in a 3D virtual space.

- ✓ No need to carry extra weight, it is in your personal computer.
- ✓ Never run out of C atoms, or any atom, your atom-box is endless.
- ✓ Place the atoms at will not constrained by certain angles and lengths.
- ✓ Place them with accurate mouse pointing or by accurate coordinates input.
- ✓ Customize, radii and colors of atoms and bonds.
- ✓ Store and classify in several effective ways all our created molecular models.
- ✓ Share by email (for example), import models from your friends.
- ✓ Import models from standard data bases of molecules.
- ✓ Combine old models easily, cut them, paste them, duplicate them
- ...
- ✓ **Go way beyond molecular modeling and displaying:**
 - ✓ Model periodic structures (crystals, surfaces, wires)
 - ✓ Click to recalculate and display all bonds at once
 - ✓ Click to trigger a quantum mechanical calculation that will give results for your model:
 - ✓ Its chemical stability
 - ✓ Its mechanical properties (elasticity, hardness)
 - ✓ Its electronic density (molecular orbitals, crystal orbitals)
 - ✓ Its motion, its vibrations with temperature.
 - ✓ Its magnetic properties
 - ✓ Etc (Electronic transport, band structures, ... all the way to professional level accuracy and details)



About Atelgraphics

Atelgraphics is a young company, founded in 2013, that recently became a member of the *Science Park of Madrid* (www.fpcm.es) the major incubator of edge-technology-based companies supported by major public and private institutions (Universidad Autónoma de Madrid, Universidad Complutense de Madrid, Banco Santander, CSIC, etc ...).

Atelgraphics' products are strongly based on tens of years of research in quantum physical chemistry, atomistic simulations, and software design, as performed by its funding team.

Atelgraphics has recently won, in competitive contest, several prizes including some 3 years funding by the *Spain's Ministry of Science and Technology*. Its current business phase aims to attract extra funding to be able to enhance and expand its business scope in a dynamical ever growing nanotechnology-driven market.

For more information refer to www.atelgraphics.com.



El FSE invierte en tu futuro