Jmol

an open-source Java viewer for chemical structures in 3D

with features for chemicals, crystals, materials and biomolecules

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Introducing the speaker

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Technical

- Triple formula:
  - **Jmol application** (3.7 MiB)
  - **JmolApplet** (≤1.1 MiB, modular)
  - **Systems integration component** (library, to insert Jmol into other software)
- JVM 1.4 (1.1 applet?)
- There is a signed version of the applet, but most use unsigned

www.Jmol.org

Background..

- Motivation for the project
  - XMol (molecular viewing program, Minnesota Supercomputer Center)
    - source code not available to users
    - no longer being maintained
    - free binary versions had become obsolete
  - Chime (MDL Inc.)
    - derived from RasMol (open code, Roger Sayle)
    - proprietary code
    - not updated to support new web browsers

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..Background..

- Development milestones
  - Jmol v. 1 - 9:
    - Dan Gezelter: Jmol invention, open source (an OpenScience project), as XMol replacement
    - Bradley Smith
    - Egon Willighagen; integration with The Chemistry Development Kit

J. Daniel Gezelter
U. Notre Dame, USA

Egon L. Willighagen
Radboud University
Nijmegen, The Netherlands

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..Background..

- Development milestones
  - Jmol v. 10:
    - Michael Howard (*Miguel*)
    - RasMol/Chime compatibility
    - reworked graphics engine
      - no Java2D graphics
      - software-based graphics
      - no specialized graphics hardware
      - up to 10^5 atoms (Java memory is the limit)
    - separate modules (e.g. file I/O)
    - feedback from users; expansion
    - v. 10.0 released on Dec.2004 (10.2 Apr.06)

Michael T. Howard
USA

www.Jmol.org

..Background


Robert M. Hanson
St. Olaf College, USA

- Development milestones
  - Jmol v. 11:
    - Bob Hanson
    - expanded functionality
    - broader coverage for multiple disciplines
      - organic
      - inorganic
      - materials
      - object drawing
      - mesh & iso-surfaces
      - bio(macro)molecules
      - crystallography
      - nanostructures
      - mathematical functions
      - sudoku …
    - 11.0 (Feb.07), 11.2 (Aug.07), 11.4 (Jan.08)

www.Jmol.org

Future..

- Currently, mainly driven by users' requests (and Bob's imagination)
- "Jmol math"
  - variables (atom-associated or otherwise)
    - boolean, integer, decimal, string, point, plane, atom bitset, bond bitset, array
  - operators: and or not + - * / modulus
  - custom atom properties, external data
  - conditionals and loops
    - for / end for, if / else if / else / end if, while / end while, goto
  - extract or assign information per atom

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..Future

- Some interests
  - better secondary structure assignment for proteins
  - calculate H bonds between sidechains
  - export animated images
  - a preloader applet (to advise that Jmol is on its way)
  - better documentation, maybe built-in
  - multi-user environments
  - integration in Wikipedia

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Uses of Jmol

Uses: instruction

- Tutorials for teaching
- Open investigation of molecular structures
  - Jmol app
  - FirstGlance in Jmol (Eric Martz)
- Wikis
- Moodle, WebAssign, LON-CAPA sites
- Animated reaction mechanisms

Uses: database viewer

- Viewer in databases
  - RCSB Protein Data Bank (PDB)
    - OCA Browser
    - STING Millennium
    - FirstGlance in Jmol
  - ChemExper Chemical Directory
  - Inorganic Crystal Structure Database
  - The Virtual Museum of Minerals and Molecules
  - ...
- Viewer for Folding@Home projects (Nicolas Vervelle)

Uses: enrich journals

- Journals: supplementary material for articles in papers
  - ACS Chemical Biology
  - Biochemical Journal
  - Chemical Reviews (ACS)
  - Crystallography Journals Online (IUCr)
  - Molecular BioSystems (Royal Soc. Chem.)
  - Nature Chemical Biology
  - Nature Structural & Molecular Biology
  - Inorganic Chemistry (ACS)
  - JACS
  - Journal of Chemical Education
  - Journal of Molecular Biology (soon)
  - Journal of Natural Products
  - Organic Letters

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Uses: Jmol within applications

- Bioclipse
  - integrated environment for biomolecule investigation
- CaGe
- ChemPad
  - 3D models calculated on-the-fly from a formula sketched by hand in a tablet PC
- iBabel
  - a GUI for Openbabel
- Janocchio
  - calculates NMR coupling constants and NOEs
- Molecular Workbench
- PFAAT (Protein Family Alignment Annotation Tool)
- ProteinGlimpse
- Spice
- STING Millennium
- STRAP
- Taverna

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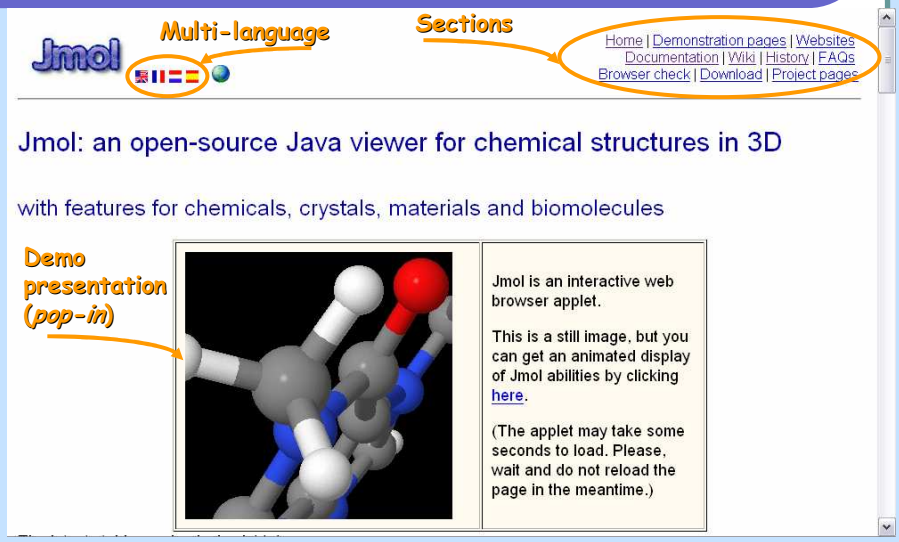
Features

Find out about features

- Web page, Wiki, scripting doc page
- Jmol web screenshots section
- Bob's test/demo pages
  - http://chemapps.stolaf.edu/jmol/ [link]
- and Presentations
  - ConfChem (spring'06) - Bob, Egon, Nicolas, Tim & Miguel [link]
  - Nature Preceedings ('07) – Egon & Miguel [link] DOI:10.1038/npre.2007.50.1

Web site



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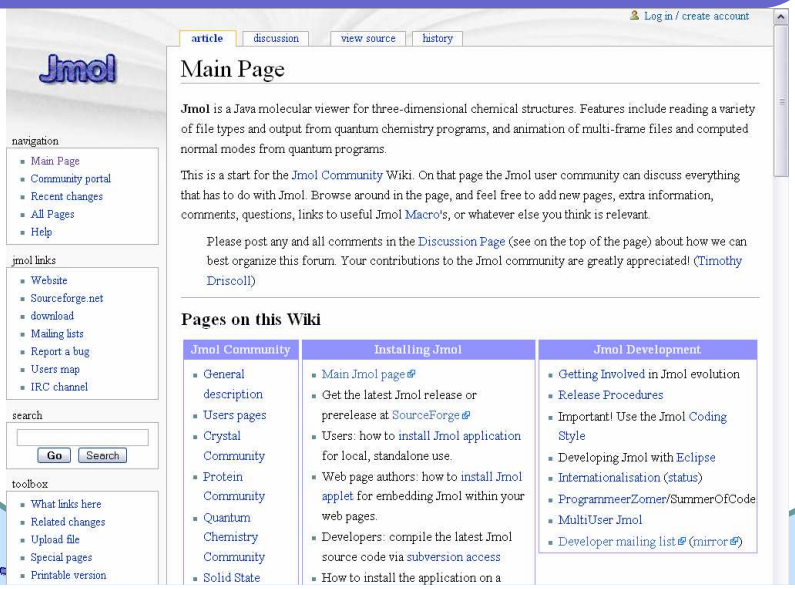
Wiki (users contribution)



www.

e-mail distribution lists

- Jmol-users
- Jmol-developers
- Jmol-commits

- access from Jmol web or project site
  - http://jmol.org
  - http://sourceforge.net/projects/jmol

File input: Jmol can read…

- CIF, mmCIF, CML, CSF, GAMESS, Gaussian, Ghemical, gOpenMol PLT, HIN, Jaguar, MOL, Molden, MOLPRO, MOPAC, NWCHEM, Odyssey, OpenDX, PDB nmrPDB, Q-Chem, SHELX, SMILES, Spartan, XYZ, XYZvib …
- Read one or several models, from one or several files
- Scripts (RasMol/Chime/Jmol), isosurfaces (Cube, jvxl), molecular orbitals
- Gzipped or zipped files
- From the clipboard
- Inline models (e.g. from web page or database)

File output: Jmol can export…

- Molecular coordinates (mol, pdb, xyz), for part of the model
- Current model state as a script
- Isosurfaces (jvxl), inc. molecular orbitals
- Command history
- Images * (png, ppm, variable jpg), PDF
- POV-Ray *
- To the clipboard
- Web pages (several templates)
- VRML, Maya (preliminary)
  - * screenshot of current view at custom size
- Custom export by adding a user's Java module

app vs. applet

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What can Jmol calculate

- Autobonding based on element and distance
  - may be disabled
- H bonds (only protein backbone and nucleic base pairs)
- Alternating single/double aromatic bonds
- Distances, angles, dihedrals
- Distance to isosurfaces
- Secondary structure in proteins
- Disulphide bonds

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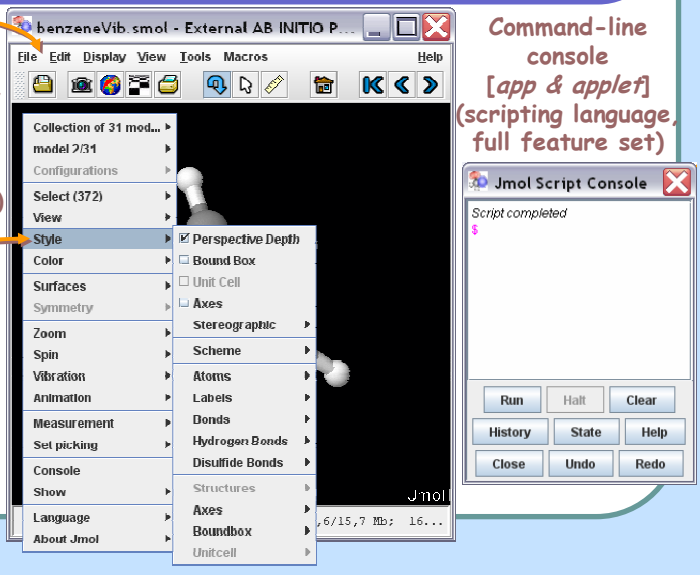
Interface

- Mouse (rotation, zoom, translation)
- GUI menus
- Command line (commands, script files)
- Web page (applet + JavaScript)

Menus and commands

Top menu
[*app only*]
(file operations, table of measurements, macros, basic rendering)

Pop-up menu
[*app & applet*]
(more powerful)



Command-line console
[*app & applet*]
(scripting language, full feature set)

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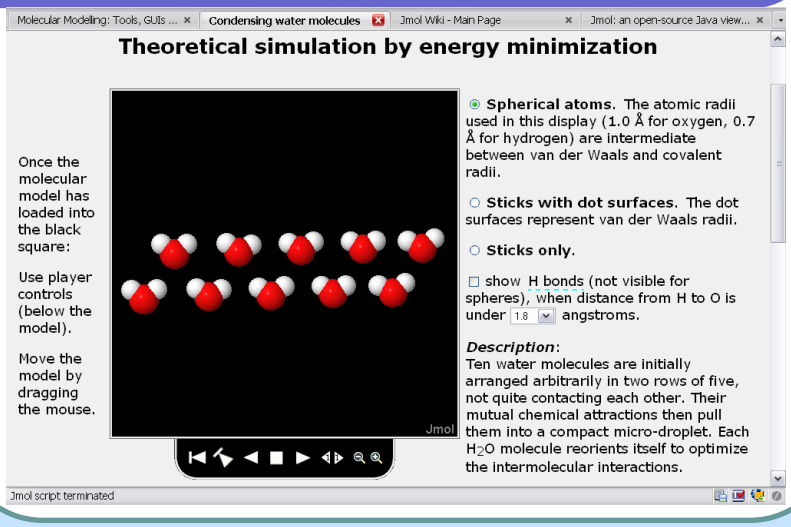
Controls in web page (JavaScript)



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Custom interface

- Internationalised & localised:
  - English, Spanish, French, German, Dutch, Portuguese, Brazilian, Czech, Turkish, Catalan, Estonian
  - defaults to system language
  - other language can be forced on-the-fly
  - even error messages
- Pop-up menu may be disabled
- Customisable pop-up menus

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Crystallography

Crystals

- Reads unit cell, symmetry and lattice information
- Handles fractional coordinates
- Manages crystallographic symmetry
  - loads a range of unit cells
  - determines the symmetry operations for a file
  - generates and fills extra unit cells
  - selects atoms based on distance from a plane
- Space groups and unit cells may be defined from any file format
- Planar slices through a model based on Miller index planes
- Extended options for unit cell and boundbox

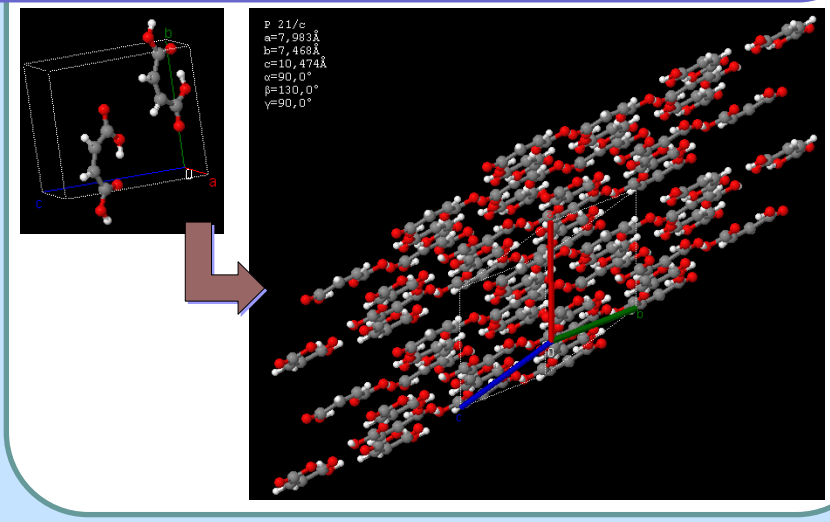
www.Jmol.org

XTALX - Jmol Crystal Explorer

- Bob Hanson
- http://fusion.stolaf.edu/chemistry/jmol/xtalx/
  - search a database (either RCSB or the American Mineralogist Crystal Structure Database),
  - or enter the URL for any uncompressed model,
  - or select a model from the list,
  - or paste or edit file data here.
  - click on 'a' or 'b' or 'c' to see more unit cells

www.Jmol.org

load "maleic.cif" 3 {2,2,2}; set showUnitCell on



www.Jmol.org

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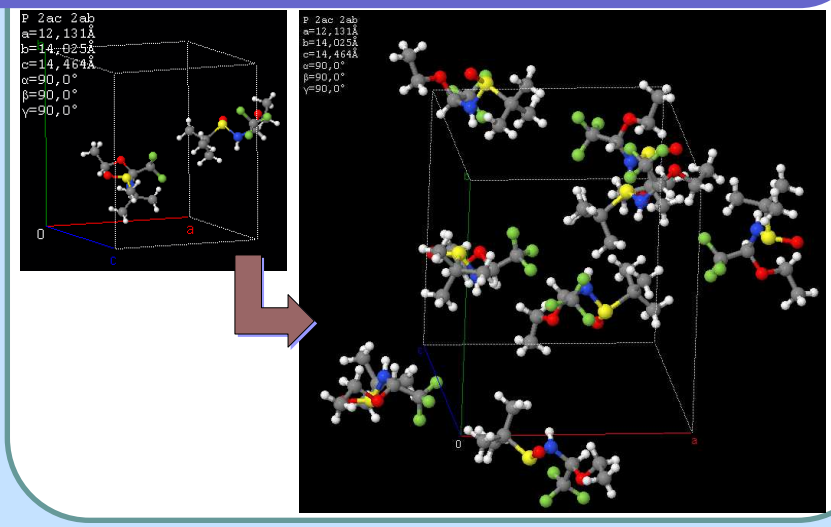

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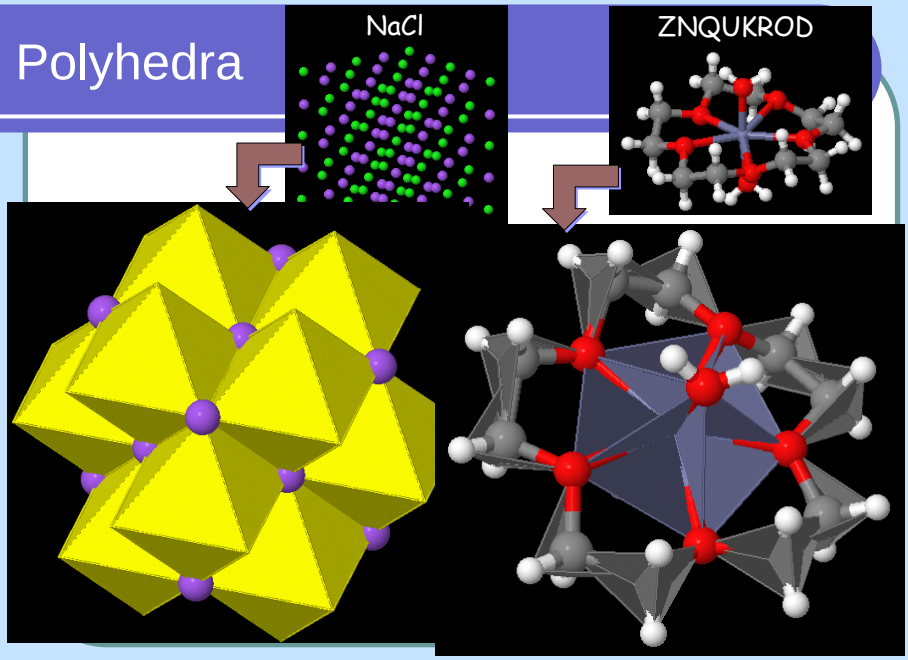
Polyhedra



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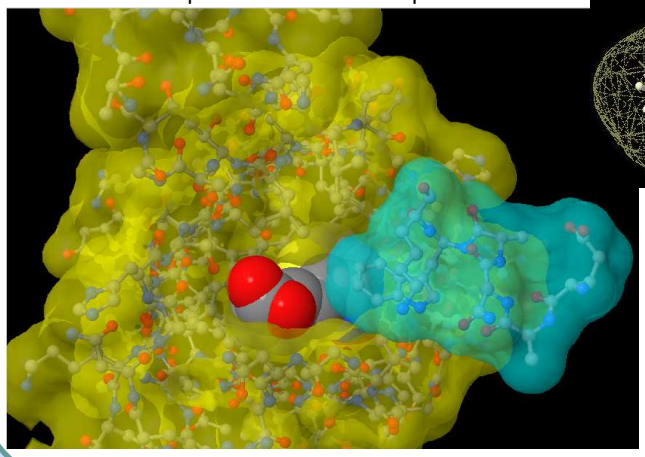
Surfaces

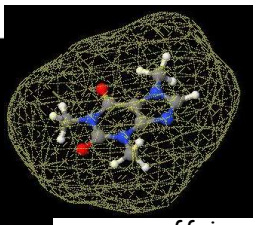
Surface types

- pMesh
  - geometric data from file
- isoSurface
  - molecular data from file (Gaussian Cube, molecular orbitals, "Jmol voxel" jvxl)
  - calculated by Jmol
  - may be used for colouring (e.g., by electrostatic potential)
  - may be calculated using user's radii
  - style: dots / mesh / solid

Molecular/solvent surfaces

biotin bound to its pocket between 2 streptavidin subunits





caffeine

- SAS
- SES
- custom probe size

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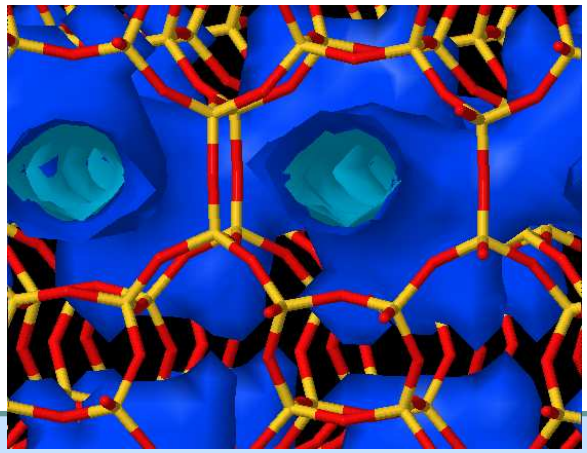
Cavities

- Database of Zeolite Structures
  http://www.iza-structure.org/databases/



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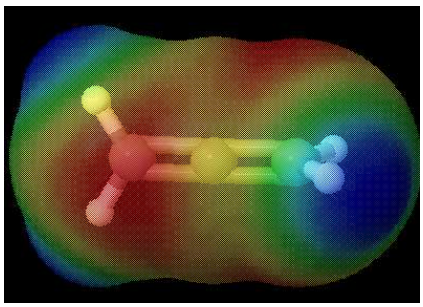
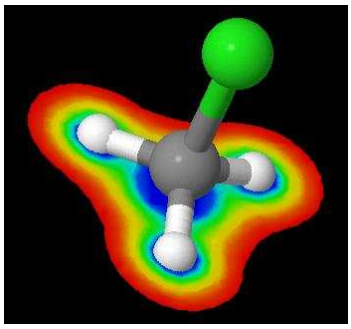
Electrostatic potentials



Mapped onto an isosurface

Bob Hanson



- User-settable charges for MEP calculation

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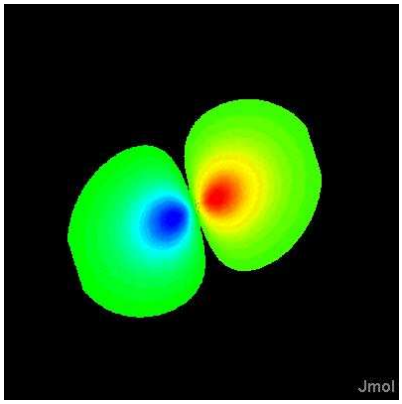
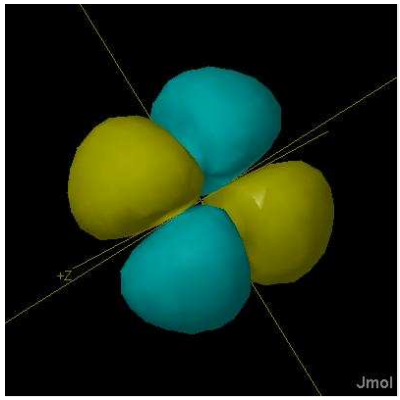
Atomic orbitals



Bob Hanson



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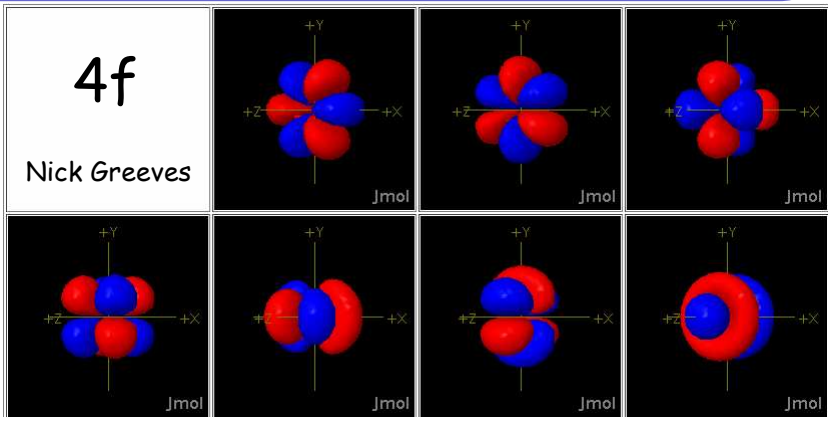
Atomic orbitals



- Support for spherical and cartesian d and f orbital basis sets

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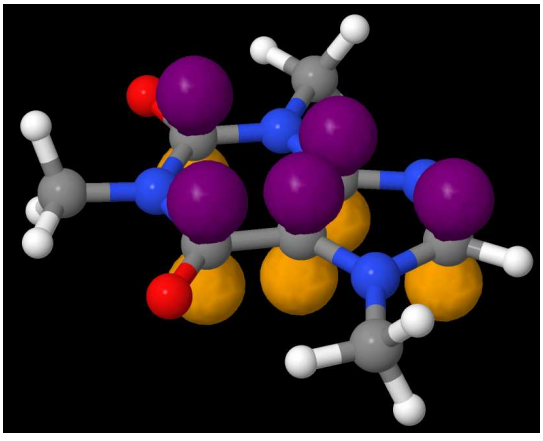
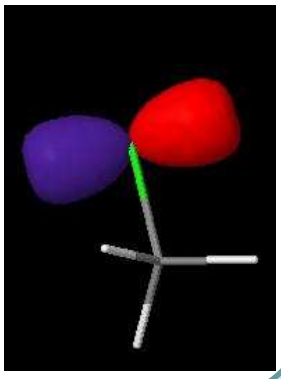
LCAO “cartoons”



Bob Hanson



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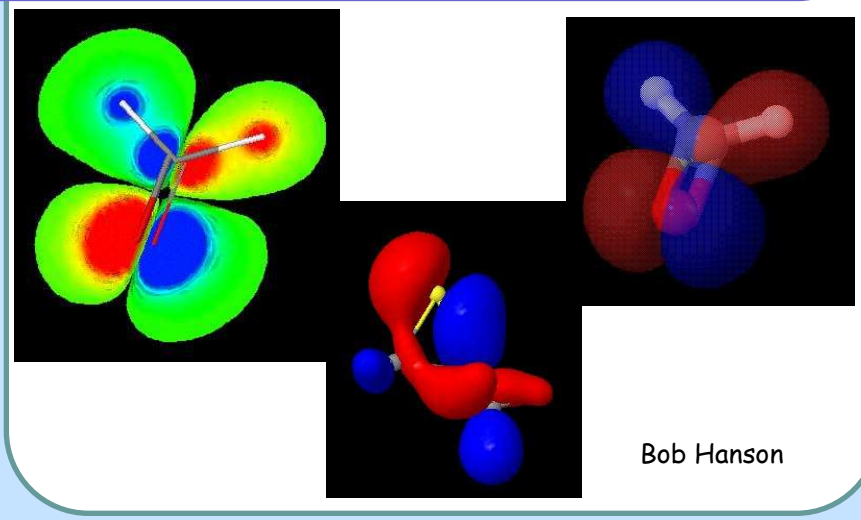
Molecular orbitals



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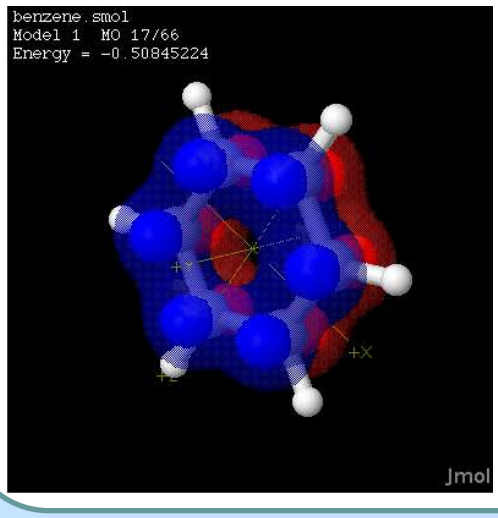
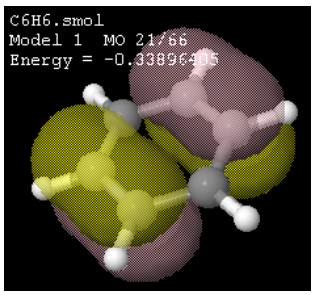
Molecular orbitals





Nick Greeves

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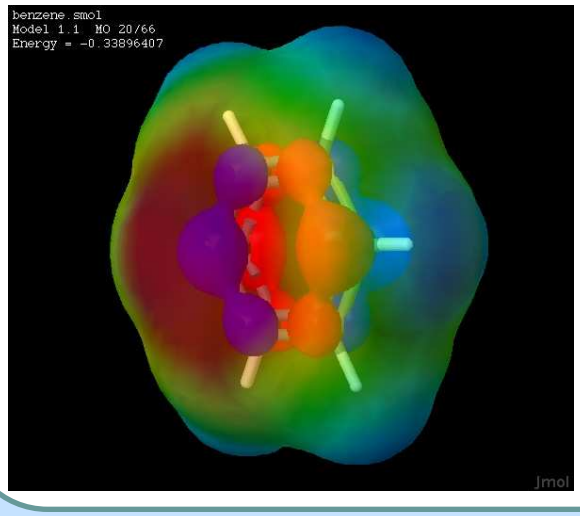
Molecular orbitals



molecular orbital + molecular surface

Nick Greeves

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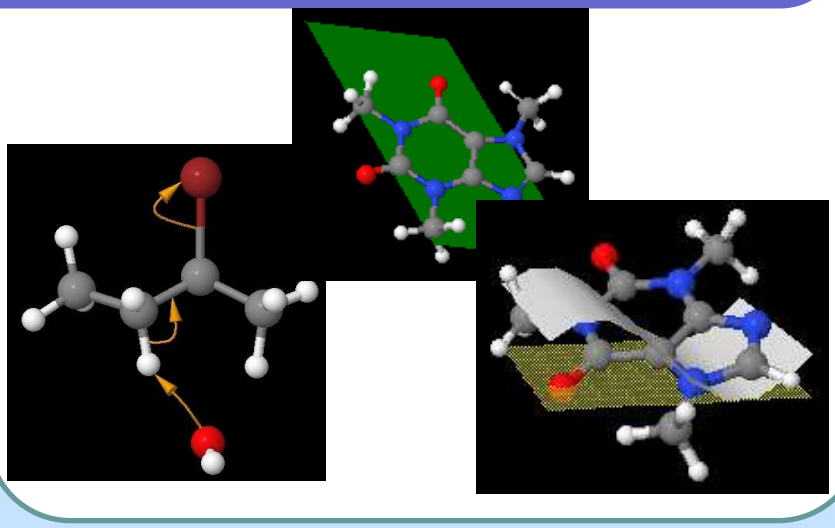
Lines, arrows, planes, mesh surfaces



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Ellipsoids, user-defined functions

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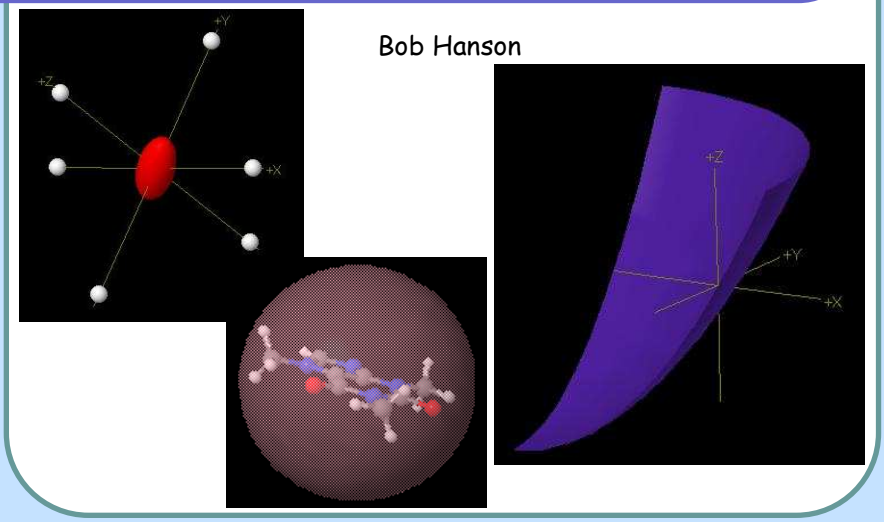

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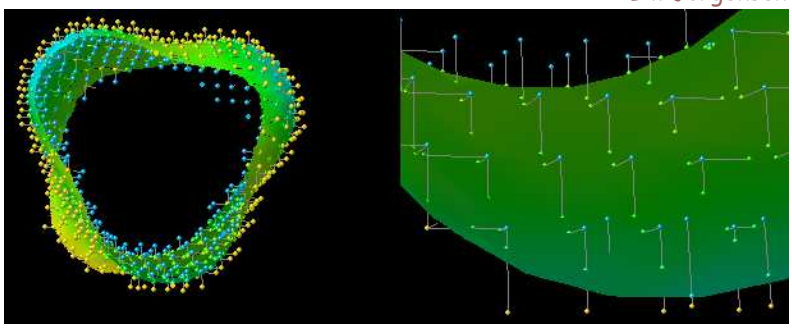
Isosurface implementation

- Adapted Marching Cubes algorithm
- Marching Squares algorithm
- Dynamic cube generation
- Read/write JVXL file format

Bob Hanson
Miguel Howard
Olaf Hall-Holt
Won Kyu Park
Daniel Severance
Bill Jorgensen



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Models in movement

Moving models: animations

- Save (to memory) and restore model orientation and state
- Scripted movement of the model
  - translation + rotation + zoom
- Multiple models in one or several files
  - conformational change
  - reaction intermediates
    - (Nick Greeves, www.ChemTube3D.com)
- Vibration
  - associated to frequencies
  - animated vibration and vectors

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Vibration

- Shows vibration direction and amplitude as 3D arrows
- Shows vibration as animation
- List of frequencies (for multimodel files with a vibration in each frame)

- Demo

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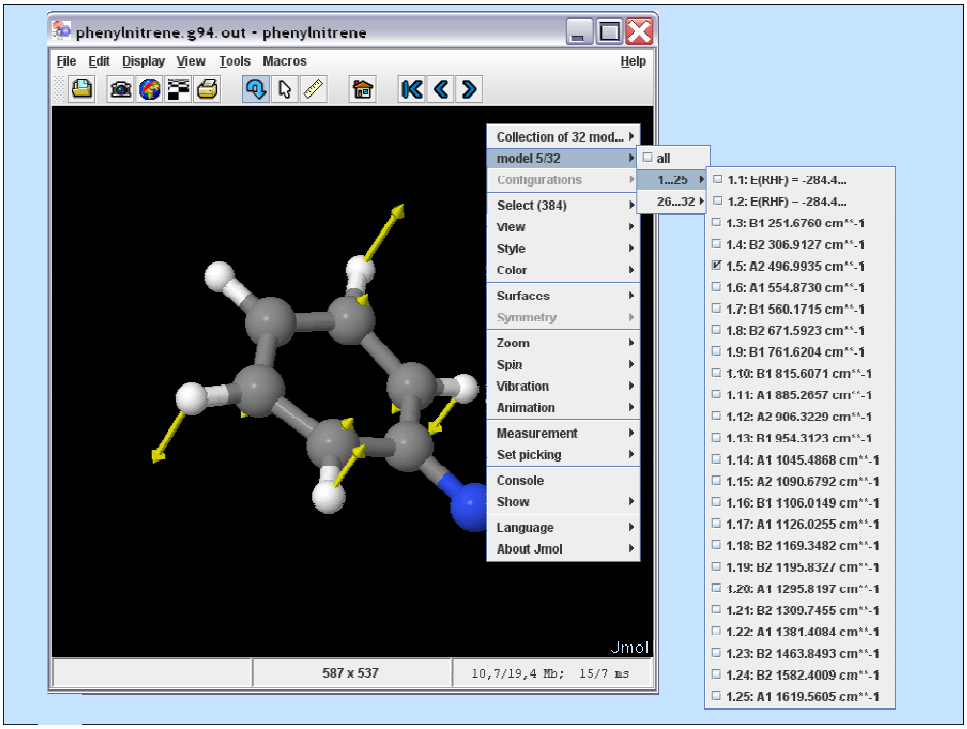

Miscellanea

Improved image quality

- Smoothing of ribbons
- Partial translucency (8 levels, several layers)
- Antialiasing for display and for export
- Export to POV-Ray
  - http://chemapps.stolaf.edu/jmol/docs/examples-11/povray.htm
- Export to Maya and VRML

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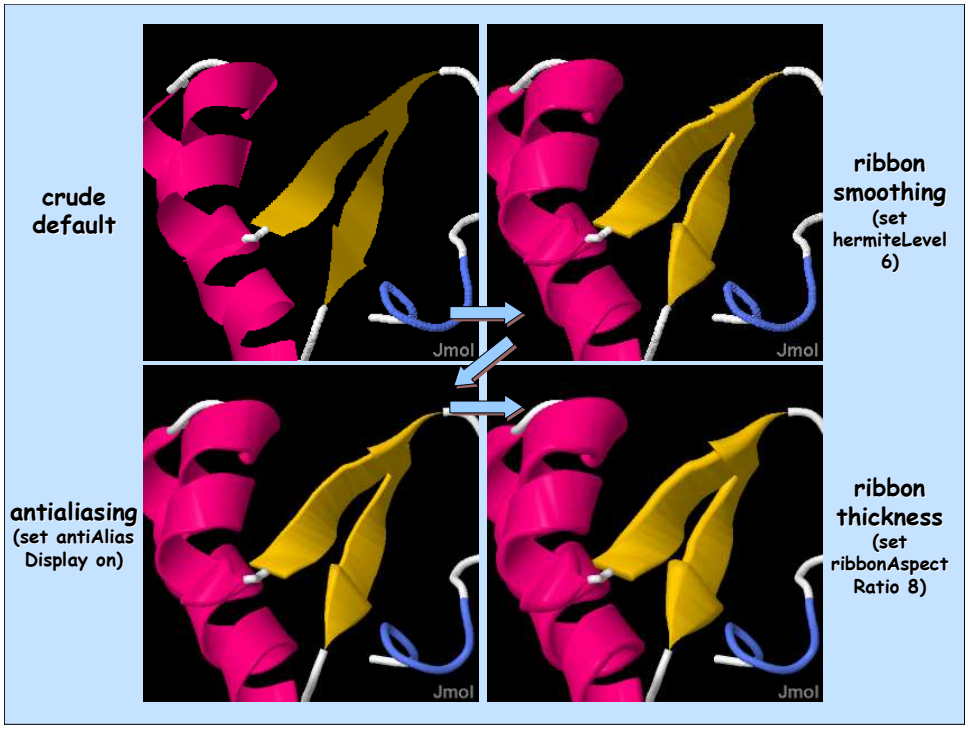
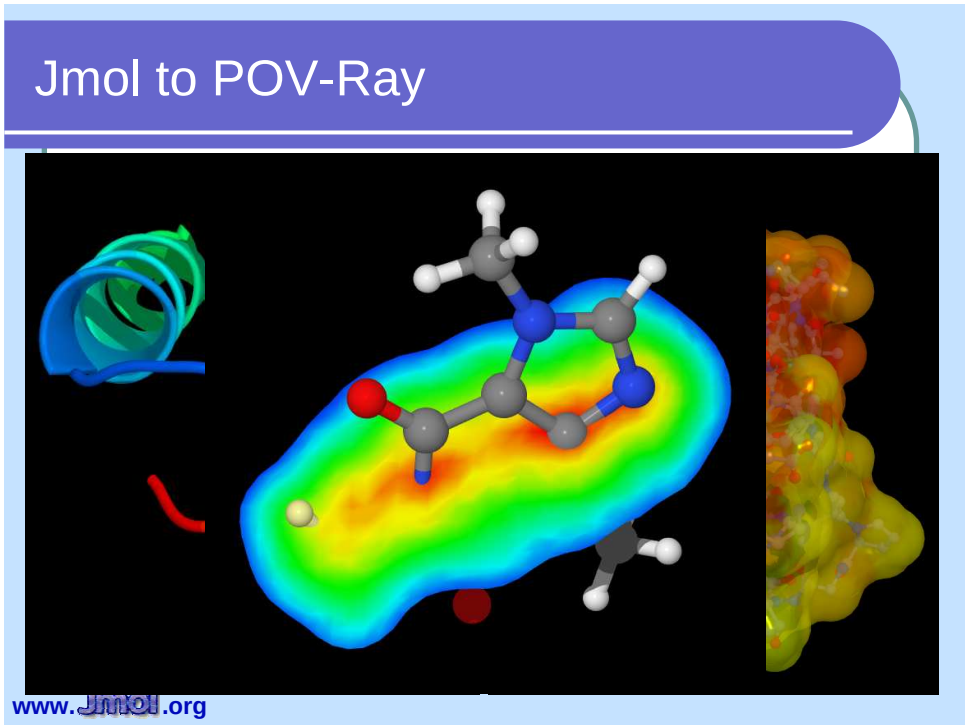

crude default
ribbon smoothing (set hermiteLevel 6)
antialiasing (set antiAlias Display on)
ribbon thickness (set ribbonAspect Ratio 8)
Jmol
Jmol
Jmol
Jmol


Jmol to POV-Ray
www.Jmol.org

Limited model edition

- Bonds can be created, modified or deleted
  - single, multiple, aromatic and several types of partial bonds
- Atoms can be moved
- Translation, rotation, spinning, and point/plane inversion of selected atoms
- Atoms can be added
- Atom properties can be set directly using Jmol math or with an array

Annotation

- Atom labels, group labels, frame labels
  - label frame and pointer
- Crystallographic information
- Free text ("echo")
  - positioned in 2D or 3D
  - multi-line
  - font control: face, size, style, colour
  - Unicode character support
  - may act as hyperlink

More

- Slab and depth planes (cut through the model)
  - world coordinates or model coordinates
- Stereo
  - side-by-side: cross-eyed, wall-eyed, custom angle
  - anaglyphic: red-blue, red-cyan, red-green, custom
- Perspective: orthogonal or conical
- Synchronization of several applets
- "Navigation" mode (fly through the model)
- Interactive Ramachandran plots

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Acknowledgements

- Jmol developers
  - Miguel Howard (lead programmer)
  - Bob Hanson (lead programmer)
  - Egon Willighagen (programmer and integration)
  - Nicolas Vervelle (web, localisation, packaging and release)
  - Daniel Leidert (localisation)
  - Jonathan Gutow (web export)
  - Pim Schravendijk (wiki, POV-Ray)
  - Bradley Smith (programmer)
  - Dan Gezelter (lead programmer)
  - yours truly (web, doc., templates)
- Expert users / testers / advisors
  - Hens Borkent
  - Patrick Carroll
  - Tim Driscoll
  - Nick Greeves
  - Alan Hewat
  - Rolf Huehne
  - Eric Martz
  - Karl Oberholser
  - Paul Pillot
  - Frieda Reichsman
  - Henry Rzepa
  - Richard Spinney
  - Steven Spilatro
  - Oliver Stueker
  - many others…

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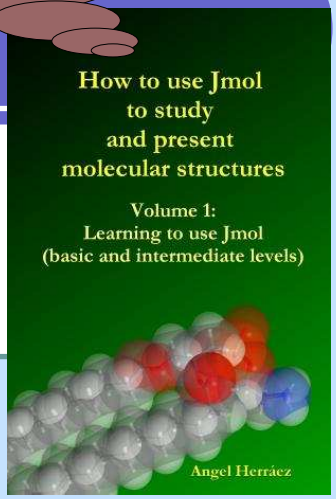
Oops! Finally, the advertising
ISBN 978-1-84799-259-8
(just use the link in my website)

Thank you!

angel.herraez@uah.es
http://biomodel.uah.es/
Google "angel herraez"



Some links

- www.jmol.org/ Web site
- wiki.jmol.org/ Wiki
- chemapps.stolaf.edu/jmol/ Bob's demos
- biomodel.uah.es/Jmol/
  Angel's Jmol (technical) pages
- www.iza-structure.org/databases/
  Database of Zeolite Structures
- www.ChemTube3D.com/
  Organic reaction mechanisms
- firstglance.jmol.org/ FirstGlance in Jmol
- Presentations on Jmol:
  - http://chemapps.stolaf.edu/jmol/presentations/confchem2006/jmol-confchem.htm
  - http://precedings.nature.com/documents/50/version/1

www.Jmol.org

Some links

- Early articles about chemistry visualisation in the web:
  - **Chemical applications of the World-Wide-Web system**. Rzepa, Whitaker & Winter (1994) J. Chem. Soc., Chem. Commun. 1944, 1907-1910, doi: 10.1039/C39940001907
  - **Hyperactive molecules and the World-Wide-Web information system**. Casher, Chandramohan, Hargreaves, Leach, Murray-Rust, Rzepa, Sayle & Whitaker (1995). J. Chem. Soc. Perkin Trans. 2, 7-11, doi: 10.1039/P29950000007

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