

# Surfaces and Orbitals

**Talk to a Teacher**

<http://spoken-tutorial.org>

**National Mission on Education through ICT**

<http://sakshat.ac.in>

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# Learning Objectives



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- ▶ Create models of alicyclic and aromatic molecules



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- ▶ **Create models of alicyclic and aromatic molecules**
- ▶ **Display different surfaces of molecules**



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- ▶ **Create models of alicyclic and aromatic molecules**
- ▶ **Display different surfaces of molecules**
- ▶ **Display atomic and molecular orbitals**



# Pre-requisites

You should know how to



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- ▶ Create and edit molecular models in Jmol Application



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You should know how to

- ▶ Create and edit molecular models in Jmol Application
- ▶ If not, watch the relevant tutorials available at <http://spoken-tutorial.org>



# System Requirements



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- ▶ **Ubuntu OS version 12.04**



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- ▶ **Jmol version 12.2.2**



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- ▶ **Jmol version 12.2.2**
- ▶ **Java (JRE) version 7  
(Sun Microsystems)**

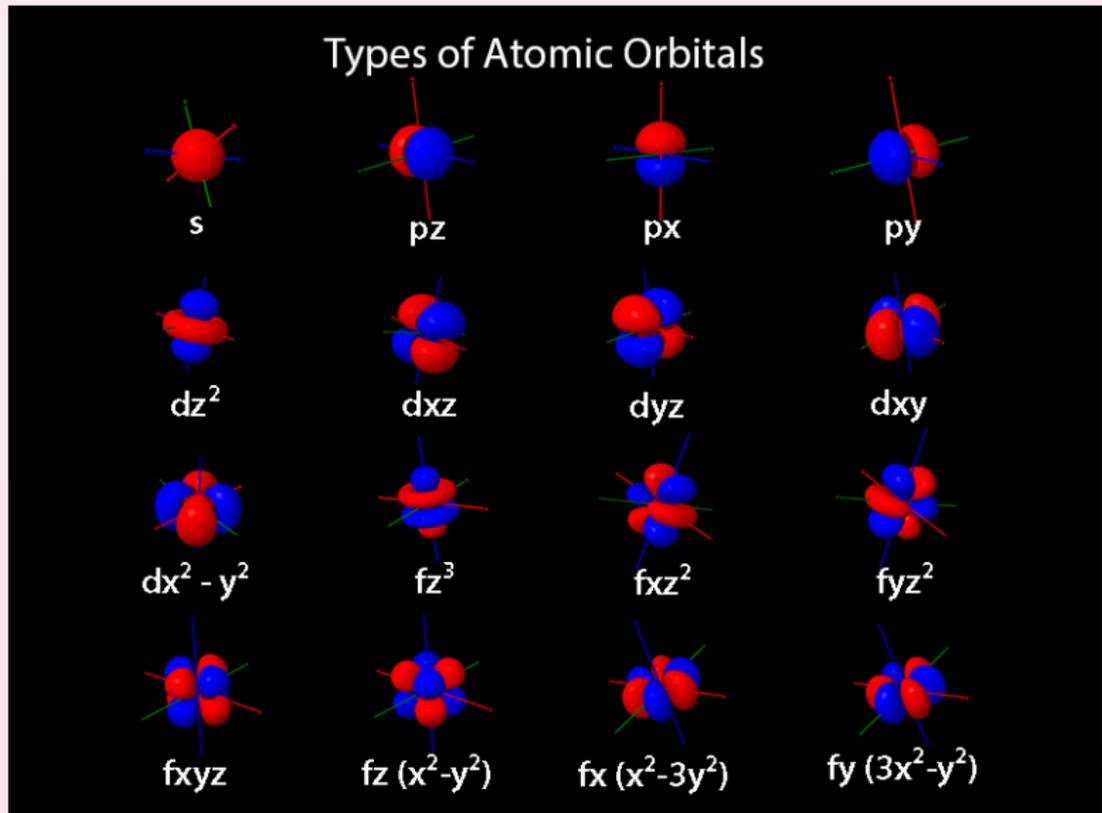


# Script Commands

Type of orbital	Script command
	<b>\$ command line n l m</b>
s	\$ isosurface phase atomicorbital 2 0 0
px	\$ isosurface phase atomicorbital 2 1 0
py	\$ isosurface phase atomicorbital 2 1 1
pz	\$ isosurface phase atomicorbital 2 1 -1
dz <sup>2</sup>	\$ isosurface phase atomicorbital 3 2 0
dxz	\$ isosurface phase atomicorbital 3 2 1
dyz	\$ isosurface phase atomicorbital 3 2 -1
dxy	\$ isosurface phase atomicorbital 3 2 2
d(x <sup>2</sup> -y <sup>2</sup> )	\$ isosurface phase atomicorbital 3 2 -2
fx <sup>3</sup>	\$ isosurface phase atomicorbital 4 3 0
fxz <sup>2</sup>	\$ isosurface phase atomicorbital 4 3 1
fyz <sup>2</sup>	\$ isosurface phase atomicorbital 4 3 -1
fxyz	\$ isosurface phase atomicorbital 4 3 2
fz(x <sup>2</sup> -y <sup>2</sup> )	\$ isosurface phase atomicorbital 4 3 -2
fx(x <sup>2</sup> -y <sup>2</sup> )	\$ isosurface phase atomicorbital 4 3 3
fy(x <sup>2</sup> -y <sup>2</sup> )	\$ isosurface phase atomicorbital 4 3 -3



# Types of Atomic Orbitals



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# Molecular Orbitals



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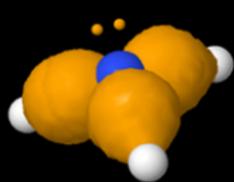
# Molecular Orbitals

- ▶ **Linear Combination of Atomic Orbitals (LCAO) method is used to create Molecular Orbitals**
- ▶ **The Command line to create Molecular Orbitals:**  
*lcaocartoon create*

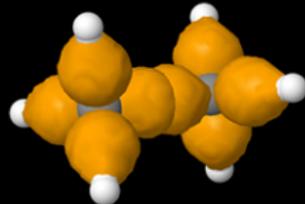


# Types of Molecular Orbitals

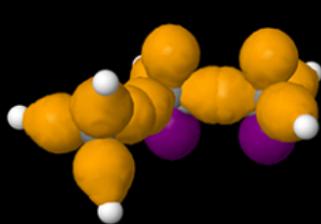
## Types of Molecular Orbitals



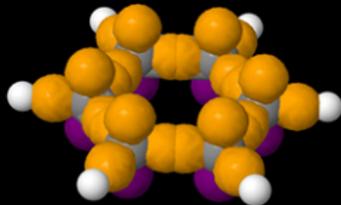
Ammonia -  $sp^3$



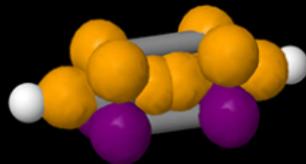
Ethane -  $sp^3$



Propene -  $sp^2$



Benzene -  $sp^2$



Ethyne -  $sp$



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# Summary

- ▶ **Create a model of cyclohexane and cyclopentane**
- ▶ **Create a model of benzene**
- ▶ **Display surface topology of molecules**



# Summary

- ▶ **Display atomic orbitals**  
*s, p, d and f*
- ▶ **Display molecular orbitals**  
*sp<sup>3</sup>, sp<sup>2</sup> and sp*



# Assignment

- ▶ Create a model of 2-butene and display molecular orbitals
- ▶ Explore `lcaocartoon` command to change the color and size of molecular orbitals
- ▶ <http://chemapps.stolaf.edu/jmol/docs/>



# About the Spoken Tutorial Project

- ▶ Watch the video available at [http://spoken-tutorial.org/What\\_is\\_a\\_Spoken\\_Tutorial](http://spoken-tutorial.org/What_is_a_Spoken_Tutorial)
- ▶ It summarises the Spoken Tutorial project



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- ▶ It summarises the Spoken Tutorial project
- ▶ If you do not have good bandwidth, you can download and watch it



# Spoken Tutorial Workshops

## The Spoken Tutorial Project Team

- ▶ Conducts workshops using spoken tutorials
- ▶ Gives certificates to those who pass an online test
- ▶ For more details, please write to [contact@spoken-tutorial.org](mailto:contact@spoken-tutorial.org)



# Acknowledgements

- ▶ Spoken Tutorial Project is a part of the Talk to a Teacher project
- ▶ It is supported by the National Mission on Education through ICT, MHRD, Government of India
- ▶ More information on this Mission is available at

<http://spoken-tutorial.org/NMEICT-Intro>

