Unified molecular orbital images for the chemistry classroom

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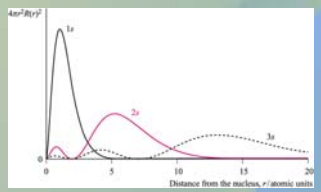
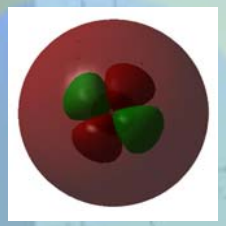
Abstract: Molecular orbital (MO) theory is the underlying concept behind chemical bonding and reactions, which is of utmost importance to the inorganic and physical chemist. Students traditionally have difficulties comprehending MO theory and its application to the linear combination of atomic orbitals. To address this issue, we have developed a unified set of molecular and atomic orbital images for use in the chemistry classroom. These images give the student a better conceptual understanding of three-dimensional orbitals than routinely used representations. The images illustrate inner nodal planes, shielding, and step-by-step formation of MOs. Static pictures were generated using commercially available and free software tools. We have also begun efforts to create animated sequences illustrating the process of MO formation.

Shielding: Core orbitals shield nuclear attractive forces from the outer shell electrons

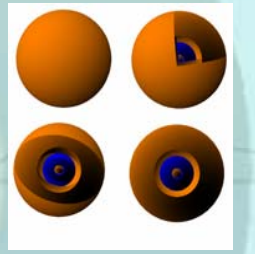


Picture illustrating shielding in one of today's inorganic texts (Housecroft, Sharpe)

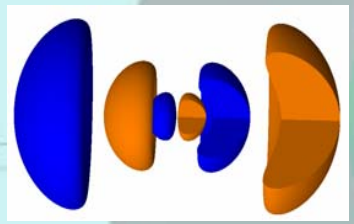


Our image: The 3d orbitals shield the outer 4s orbital

Cut-away Images: Sequences of cut-away orbital images allow students to see the orbital shape as well as the inner nodes

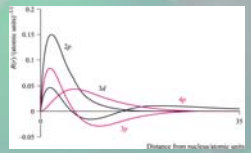


Progression of a 4s orbital, illustrating both the spherical shape and radial nodes

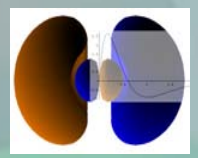


Cutaway of a 4p orbital, showing the rounded shape of each nodal plane

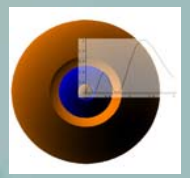
Wavefunction mapping: Radial wavefunctions and probability curves are mapped onto orbital plots



Picture illustrating wavefunctions and nodes in a modern inorganic text (Housecroft, Sharpe)

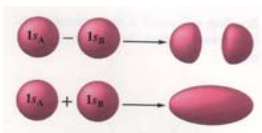


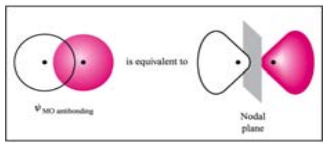
Our plot of a 3p orbital and its wavefunction.

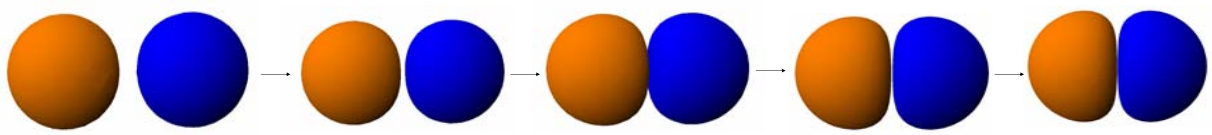


Probability plot for a 3s orbital. The electron is found more often in the outer region.

MO Formation: We used Macromedia Flash to generate animations showing the linear combination of atomic orbitals to form molecular orbitals. Standard textbook images (top left – Zumdahl, top right – Housecroft, Sharpe) are compared to our animation.





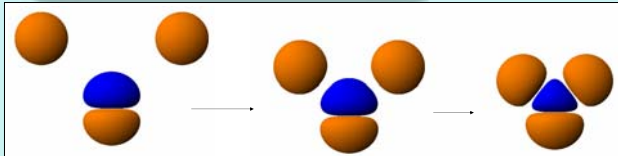


6 Angstroms | 5 Angstroms | 4 Angstroms | 3 Angstroms | 2 Angstroms

Sources:

- Orbital Viewer – © David Manthey (2004), used to generate cut-away images and pictures for animations. Surfaces drawn are of constant probability $\psi^2=10^{-4}$.
- GaussView 03W – © Gaussian Inc. (2003), used to illustrate core shielding. Surfaces at constant probability of $\psi^2=0.02$
- Macromedia Flash MX – © Macromedia Inc. (2005), used to animate and publish our images

Funding was provided by a grant from Ithaca College



Combination of hydrogen LGOs and oxygen's 2p orbital to form an antibonding orbital in water

Stop by for a demo of our animations!