An **atomic orbital** is a mathematical function that describes the wave-like behavior of either one electron or a pair of electrons in an atom.[1] This function can be used to calculate the probability of finding any electron of an atom in any specific region around the atom’s nucleus. The term may also refer to the physical region where the electron can be calculated to be, as defined by the particular mathematical form of the orbital.[2]

Atomic orbitals are typically categorized by $n$, $l$, and $m$ quantum numbers, which correspond to the electron’s energy, angular momentum, and an angular momentum vector component, respectively. Each orbital is defined by a different set of quantum numbers ($n$, $l$, and $m$), and contains a maximum of two electrons each with their own spin quantum number. The simple names **s orbital**, **p orbital**, **d orbital** and **f orbital** refer to orbitals with angular momentum quantum number $l = 0$, 1, 2 and 3 respectively. These names indicate the orbital shape and are used to describe the electron configurations. They are derived from the characteristics of their spectroscopic lines: sharp, principal, diffuse, and fundamental, the rest being named in alphabetical order (omitting j).[3][4]

Atomic orbitals are the basic building blocks of the **atomic orbital model** (alternatively known as the electron cloud or wave mechanics model), a modern framework for visualizing the microscopic behavior of electrons in matter. In this model the electron cloud of a multi-electron atom may be seen as being built up (in approximation) in an electron configuration that is a product of simpler hydrogen-like atomic orbitals. The repeating **periodicity** of the blocks of 2, 6, 10, and 14 elements within sections of the periodic table arises naturally from the total number of electrons which occupy a complete set of **s**, **p**, **d** and **f** atomic orbitals, respectively.

The shapes of the first five atomic orbitals: 1s, 2s, 2p_x, 2p_y, and 2p_z. The colors show the wave function phase. These are graphs of $\psi(x,y,z)$ functions which depend on the coordinates of one electron. To see the elongated shape of $\psi(x,y,z)^2$ functions that show probability density more directly, see the graphs of d-orbitals below.

**Shapes of orbitals**
Cross-section of computed hydrogen atom orbital ($\psi(r,\theta,\phi)^2$) for the 6s ($n=6$, $l=0$, $m=0$) orbital. Note that s orbitals, though spherically symmetrical, have radially placed wave-nodes for $n > 1$. However, only s orbitals invariably have a center anti-node; the other types never do.

Simple pictures showing orbital shapes are intended to describe the angular forms of regions in space where the electrons occupying the orbital are likely to be found. The diagrams cannot, however, show the entire region where an electron can be found, since according to quantum mechanics there is a non-zero probability of finding the electron anywhere in space. Instead the diagrams are approximate representations of boundary or contour surfaces where the probability density $|\psi(r,\theta,\phi)|^2$ has a constant value, chosen so that there is a certain probability (for example 90%) of finding the electron within the contour. Although $|\psi|^2$ as the square of an absolute value is everywhere non-negative, the sign of the wave function $\psi(r,\theta,\phi)$ is often indicated in each subregion of the orbital picture.

Sometimes the $\psi$ function will be graphed to show its phases, rather than the $|\psi(r,\theta,\phi)|^2$ which shows probability density but has no phases (which have been lost in the process of taking the absolute value, since $\psi(r,\theta,\phi)$ is a complex number). $|\psi(r,\theta,\phi)|^2$ orbital graphs tend to have less spherical, thinner lobes than $\psi(r,\theta,\phi)$ graphs, but have the same number of lobes in the same places, and otherwise are recognizable. This article, in order to show wave function phases, shows mostly $\psi(r,\theta,\phi)$ graphs.

The lobes can be viewed as interference patterns between the two counter rotating "$m$" and "-m" modes, with the projection of the orbital onto the xy plane having a resonant "m" wavelengths around the circumference. For each $m$ there are two of these $<m>+<m>-$ and $<m>-<m>$. For the case where $m=0$ the orbital is vertical, counter rotating information is unknown, and the orbital is z-axis symmetric. For the case where $l=0$ there are no counter rotating modes. There are only radial modes and the shape is spherically symmetric. For any given $n$, the smaller $l$ is, the more radial nodes there are. Loosely speaking $n$ is energy, $l$ is analogous to eccentricity, and $m$ is orientation.

Generally speaking, the number $n$ determines the size and energy of the orbital for a given nucleus: as $n$ increases, the size of the orbital increases. However, in comparing different elements, the higher nuclear charge, $Z$, of heavier elements causes their orbitals to contract by comparison to lighter ones, so that the overall size of the whole atom remains very roughly constant, even as the number of electrons in heavier elements (higher $Z$) increases.

Also in general terms, $l$ determines an orbital's shape, and $m$ its orientation. However, since some orbitals are described by equations in complex numbers, the shape sometimes depends on $m$ also.

The single s-orbitals ($l = 0$) are shaped like spheres. For $n = 1$ the sphere is "solid" (it is most dense at the center and fades exponentially outwardly), but for $n = 2$ or more, each
single s-orbital is composed of spherically symmetric surfaces which are nested shells (i.e., the "wave-structure" is radial, following a sinusoidal radial component as well). See illustration of a cross-section of these nested shells, at right. The s-orbitals for all \( n \) numbers are the only orbitals with an anti-node (a region of high wave function density) at the center of the nucleus. All other orbitals (p, d, f, etc.) have angular momentum, and thus avoid the nucleus (having a wave node at the nucleus).

The three p-orbitals for \( n = 2 \) have the form of two ellipsoids with a point of tangency at the nucleus (the two-lobed shape is sometimes referred to as a "dumbbell"). The three p-orbitals in each shell are oriented at right angles to each other, as determined by their respective linear combination of values of \( \ell \).

Four of the five d-orbitals for \( n = 3 \) look similar, each with four pear-shaped lobes, each lobe tangent to two others, and the centers of all four lying in one plane, between a pair of axes. Three of these planes are the xy-, xz-, and yz-planes, and the fourth has the centres on the x and y axes. The fifth and final d-orbital consists of three regions of high probability density: a torus with two pear-shaped regions placed symmetrically on its z axis.

There are seven f-orbitals, each with shapes more complex than those of the d-orbitals.

For each s, p, d, f and g set of orbitals, the set of orbitals which composes it forms a spherically symmetrical set of shapes. For non-s orbitals, which have lobes, the lobes point in directions so as to fill space as symmetrically as possible for number of lobes which exist for a set of orientations. For example, the three p orbitals have six lobes which are oriented to each of the six primary directions of 3-D space; for the 5 d orbitals, there are a total of 18 lobes, in which again six point in primary directions, and the 12 additional lobes fill the 12 gaps which exist between each pairs of these 6 primary axes.

Additionally, as is the case with the s orbitals, individual p, d, f and g orbitals with \( n \) values higher than the lowest possible value, exhibit an additional radial node structure which is reminiscent of harmonic waves of the same type, as compared with the lowest (or fundamental) mode of the wave. As with s orbitals, this phenomenon provides p, d, f,
and g orbitals at the next higher possible value of $n$ (for example, 3p orbitals vs. the fundamental 2p), an additional node in each lobe. Still higher values of $n$ further increase the number of radial nodes, for each type of orbital.

The shapes of atomic orbitals in one-electron atom are related to 3-dimensional spherical harmonics. These shapes are not unique, and any linear combination is valid, like a transformation to cubic harmonics, in fact it is possible to generate sets where all the d's are the same shape, just like the $p_x$, $p_y$, and $p_z$ are the same shape.[20][21]

**Molecular orbital**

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Jump to: navigation, search
See also: Molecular orbital theory

In chemistry, a **molecular orbital** (or MO) is a mathematical function describing the wave-like behavior of an electron in a molecule. This function can be used to calculate chemical and physical properties such as the probability of finding an electron in any specific region. The term "orbital" was first used in English by Robert S. Mulliken as the English translation of Schrödinger's 'Eigenfunktion'. It has since been equated with the "region" generated with the function. Molecular orbitals are usually constructed by combining atomic orbitals or hybrid orbitals from each atom of the molecule, or other molecular orbitals from groups of atoms. They can be quantitatively calculated using the Hartree-Fock or Self-Consistent Field (SCF) methods.

**Formation of molecular orbitals**

Molecular orbitals arise from allowed interactions between atomic orbitals, which are allowed if the symmetries (determined from group theory) of the atomic orbitals are compatible with each other. Efficiency of atomic orbital interactions is determined from the overlap (a measure of how well two orbitals constructively interact with one another) between two atomic orbitals, which is significant if the atomic orbitals are close in energy. Finally, the number of molecular orbitals that form must equal the number of atomic orbitals in the atoms being combined to form the molecule.

**Molecular Orbitals**

When two hydrogen atoms come together to form the hydrogen molecule, the atomic $s$ orbitals of each atom are combined to form two molecular orbitals. One of these new orbitals is the result of the addition of the two atomic orbitals, while the other is created by a subtraction of these orbitals. In the addition, a reinforcement of the wave function occurs in the region between the two nuclei. Physically, this means the electron density
increases in the area between the two nuclei. This increase in electron density causes a corresponding increase in the attraction of each positively charged nucleus for the negatively charged overlap region. It is this increased attraction that holds the hydrogen molecule together and creates the **bonding molecular orbital**. Because the bonding molecular orbital is generated from atomic $s$ orbitals, it is called a $\sigma$ (sigma) **bonding molecular orbital**.

The molecular orbital formed by the subtraction of the two wave functions has no electron density between the nuclei of the hydrogen atoms. This lack of electron density is caused by interference between the two out-of-phase wave functions. The lack of electron density between the nuclei results in the formation of a node. With no electron density between them, the hydrogen nuclei repel each other strongly, resulting in the formation of a high-energy state called an **antibonding orbital**. Because this particular antibonding orbital is created from two atomic $s$ orbitals, it is referred to as a $\sigma^*$ **antibonding molecular orbital**. The bonding and antibonding orbitals in the hydrogen molecule are illustrated in Figure 1. Note that the plus and minus symbols in the figure refer to wave phases and not electrical charge.

![Diagram of bonding and antibonding orbitals](image)

**Figure 1**

Like electrons in atomic orbitals, electrons in bonding orbitals must have **paired spins**; that is, the electrons must be spinning in opposite directions.

An energy diagram for the formation of the hydrogen molecule and the nonformation of a helium molecule are shown in Figure 2. The two electrons in a hydrogen molecule are paired in the lower-energy $\sigma$ bonding molecular orbital. No electrons (arrows, in the figure) occupy the $\sigma^*$ antibonding orbital. As long as a molecule has more electrons in the bonding orbital than in the antibonding orbital, it will be stable. In fact, in most stable molecules, the antibonding orbitals are vacant. Helium molecules do not exist because no driving force causes the helium atoms to bond. They have the same number of bonding and antibonding electrons, and thus achieve no greater stability as a molecule.
The hydrogen molecule illustrates that a $\sigma$ bond must have a heavy electron density along an imaginary line between the two nuclei. Such a density can also exist in the end-to-end overlap of atomic $p$ orbitals. As shown in Figure 3, the heaviest electron density lies along a line between the nuclei.

The overlap of atomic $s$ orbitals with hybrid atomic orbitals and the overlap of two hybrid atomic orbitals can also result in $\sigma$ bonds.

The side-to-side overlap of atomic $p$ orbitals results in high electron density above and below an imaginary line between the nuclei. This density pattern, the $\pi$ molecular orbital, leads to the formation of a $\pi$ (pi) bond. This bond is much weaker than a $\alpha$ bond because the repulsion between the electronically unshielded nuclei leads to poor orbital overlap.
Antibonding (or anti-bonding) is a type of chemical bonding. An antibonding orbital is a form of molecular orbital (MO) that is located outside the region of two distinct nuclei. The overlap of the constituent atomic orbitals is said to be out of phase, and as such the electrons present in each antibonding orbital are repulsive and act to destabilize the molecule as a whole.

Explanation

one pair

In chemistry, a lone pair is a valence electron pair without bonding or sharing with other atoms. They are found in the outermost electron shell of an atom, so lone pairs are a subset of a molecule's valence electrons. They can be identified by examining the outermost energy level of an atom—lone electron pairs consist of paired electrons as opposed to single electrons, which may appear if the atomic orbital is not full. Electron pairs are therefore considered lone pairs if two electrons are paired but are not used in chemical bonding. Thus, the number of lone electrons plus the number of bonding electrons equal the total number of valence electrons in a compound.

Polar molecules

Examples of common household polar molecules include sugar, for instance the sucrose sugar variety. Sugars have many polar oxygen–hydrogen (-OH) groups and are overall highly polar.