the general science journal

The MCAS Electronic Structure of Atoms

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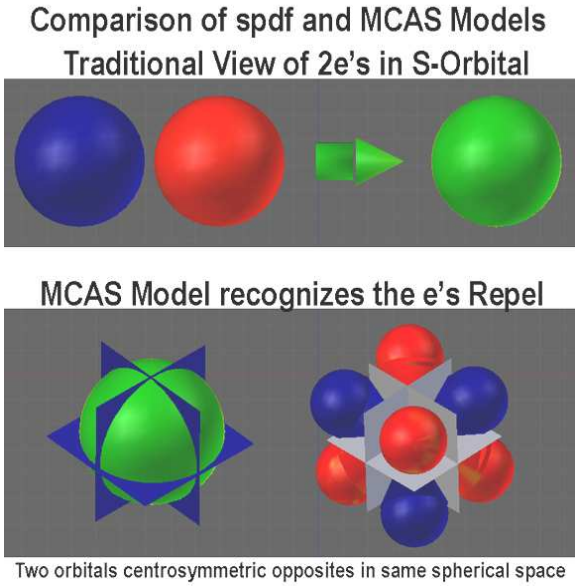
In 1999, I described the MCAS model for the electronic structure of atoms.[1] This model recognized that, while *electrons* can *exhibit duality* (wave *and* particle properties; *not or*, in our physical reality), a proper model representing them about a nucleus could not ignore their repulsive nature as the spdf model does. I represented my model with cubes as that was the imaging software I had at the time and it was easier to make paper cubes[2] than other shapes. Some thought I was proposing angular orbitals, while I was just trying to depict spatial deployment of the electron orbitals in a different way than the spdf model did. For all its claims to orthogonality, the spdf model constantly violates this premise with all those spdf orbitals occupying some of same space as similar spdf orbitals do. I have now used blender 2.61 software[3] to create tear-shaped orbitals and place them around a point, ala nucleus.

The simplest electronic orbital in the spdf model is a sphere. One electron was presumed to occupy it per the Bohr model. When a second electron was added, the two blended (paired by wave mechanics) to occupied the same spherical space – see the depiction below. Physics mathematicians made it happen and then created more elaborate arrangements. While a variety of shapes can rotate rapidly enough in our 3D space to appear as a uniform sphere, two repelling electrons would occupy "opposed positions" within that "sphere" - a point not addressed by the spdf model. A 3D xyz-grid divides the sphere into 8 equal parts (green sphere with x, y, and z planes below). These 8 can be combined into two identical, but opposing, orbital pairs having T_d-symmetry and a common center. This is the basis of the MCAS model. When each 4-lobed T_d-group contains a single electron, it is designated as an M-orbital. When the 4-lobed T_d-group contains more than one electron, it is designated as a C-orbital.



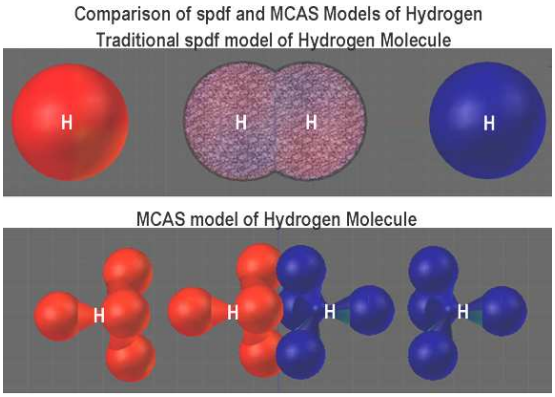
Two orbitals centrosymmetric opposites in same spherical space

[1] http://arxiv.org/html/physics/9902046v1/Article.html and http://arxiv.org/html/physics/9909053v3. First submission of the concept for publication was in 1993. Also: *The Electronic Puzzle* 1994 (LIBCONG-TXu-632-452) [cited in *A BIT TOO FAR* http://arxiv.org/html/physics/9904031]

[2] Moles, bits, and cubes, LIBCONG-TXu000593728 (1996)

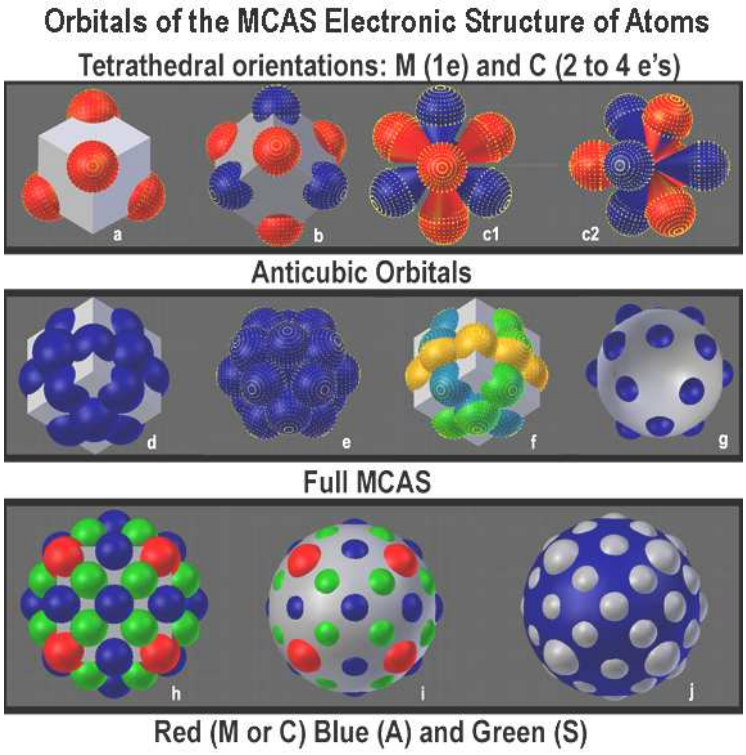
[3] www.blender.org

Before proceeding to the remaining MCAS orbitals, it is of value to see how the spdf and MCAS representations differ with regard to a simple molecule like hydrogen. In the spdf version, the spherical electron orbitals overlap with the electrons *again* blending and concentrating between the nuclei – see below. In the MCAS version, the electrons also concentrate between the nuclei, but are constrained to a single nucleus, in this case. The bond forms with each nucleus attracting the other's electron that "nest" trigonally and provide the rotational resistance observed in single bonds.



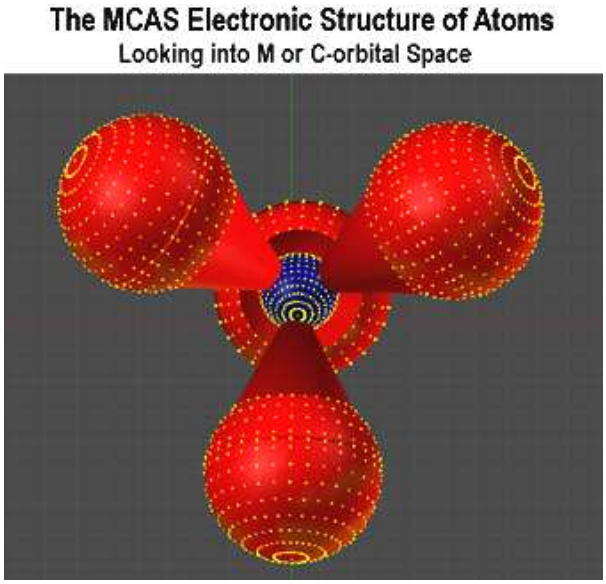
Now, for the remaining MCAS orbitals.

I originally represented the MCAS model with a cube because I find things are more easily viewed in the x,y,z-coordinates of our 3D world. The physics mathematicians apparently found this useful, too. Thus the images shown below have the single M and paired M/C orbitals with a virtual cube (a/b). When the cube is removed (images c1 and c2), the projections into space are more difficult to evaluate with the distraction of the orbital portions that go towards the nucleus. The xyz alignment is even more difficult to visualize with more orbitals. The "trigonal" symmetry as one looks down one orbital lobe (b and c1) is seen either way.



When the number of electrons is greater than M or C-orbitals can handle (relate to the reason d-orbitals were created in the spdf model), then other orbitals are needed. The most open spaces are “anticubic”. With a virtual cube present, the A (anticubic) orbitals are seen to band cubic space (d). This is less apparent in image (e) without the virtual cube. The bands in 3D are clearer when the orbitals are given different colors (f). Spatial orientation of the orbitals is more difficult to envision when the cube is replaced with a sphere (g), although the orbital outer limits are more clearly appreciated. The 18 A-orbitals match the requirement for reordering an entire level (row) in the periodic chart where 10 transition elements appear.

The next “open” symmetry after the anticube can accommodate 24 orbitals. These are depicted as the green orbitals in the above image (h) with a virtual cube. The square-face alignment which gives this orbital group its S name in the MCAS model is clearly seen. The 8 orbitals needed to make 32 for the S group are in the C-orbital directions. With a virtual sphere (i), the xyz-visualization is more difficult. Without coloration (j), just the highly symmetrical, spherical arrangement of the MCAS orbitals is seen. There are no “weird” shaped orbitals, such as the d_{z^2} orbital or the f-orbitals of the spdf model. All the electron orbital lobes of the MCAS model have the same basic shape, if not size/energy.



For more on the MCAS model and other scientific issues, see “Challenging Science” by Joel M Williams or www.swcp.com/~jmw-mcw. A number of web listings can be found by searching with MCAS modeling Joel Williams.