

# *pd*-Hybridization And The Electron Geometry Of Fluorine, Neon, And Iron

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*March 2024*

## ABSTRACT:

In this paper, the hybridization of atomic orbitals is considered through the lens of an extended relativistic quantum mechanics that we call ‘sub-quantum mechanics.’ Building upon earlier work, it is proposed that, in addition to the electrostatic driving force, the mechanisms behind electron pair formation, Pauli Exclusion, and Hund’s Second Rule are strongly influenced by the ways in which the components of electron spin affect composite atomic orbital states. These states can be either bosonic, as in the case of the *di-electron* and the proposed full shell configurations of neon and argon, or fermionic, as in the case of a hybridized boron atom. In addition, it is proposed that the repulsive interactions between *di-electron* and unpaired electron orbitals can cause the latter to become extended radially outward from an atomic valence shell. In this paper, the consequences of such a topological shift will be considered in the cases of fluorine and iron. The concept of hybridization between *p*- and *d*-orbitals, which first arises in the case of the transition metals, is also introduced. These *pd*-hybridized electron geometries may, in turn, help us to account for various elemental magnetic properties and periodic trends. Further, the specific electron geometry proposed for the iron atom may help to explain the nature and mechanism behind ferromagnetism, as well as how this mechanism might relate to both the above-mentioned orbital extension and fluorine’s very high reactivity.

## Keywords:

orbital, hybridization, spherical harmonic resonance, relativistic quantum mechanics, quantum chemistry, boron, scandium, iron, fluorine, neon, argon, ferromagnetism

## 1. INTRODUCTION

When electrons occupy the same atomic shell, they cannot ignore each others' influences, and they will resonate together into the most stable and symmetrical *single* stationary electron wave structure that they can. This means that orbitals generated via the excitation of a single electron atom can only be first approximations of the correct collective electron states of multi-electron atoms or molecules. The same is therefore true of the computational models based upon these approximations.

Hybridization states, for example  $sp^2$ ,  $sp^3$ , and  $sp^3d^2$ , have long been discussed in the context of molecular geometry. These three manifest trigonal, tetrahedral, and octahedral electron domain symmetries respectively. The forces that shape these forms may be considered to have two main aspects. The first aspect is primarily electrostatic in simple cases, although elements of electromagnetics arise as orbital spin is introduced. Electron repulsion causes orbital lobes — the structural elements within the overall wave structure that holds the electron density — to move as far apart as the atomic geometry will allow.

The second aspect lies in quantum mechanics, in general, and in quantum spin, in particular. Spin influences structure in two main ways. The first is in the overwhelming force normally referred to as the Pauli Exclusion principle, which prevents two fermions from occupying the same state. When they have ‘opposite spin’ [4], however, they not only *can* pair up, they do so most *readily*. The second force is of particular relevance here and, though weaker, may be thought of as a sort of “inclusion” principle. This is the propensity for fermions to form symmetric and spherically harmonic sets, whether as opposite-spin electrons merging into *di-electrons* (electron pairs), or when as same-spin (degenerate) electrons merging into what we might consider a single, composite fermionic state.

Paired states are denoted *di-fermions*, and are often bosonic if quantum choices are limited. Examples of this include “Cooper pair” *di-electrons* in superconductors, the *di-proton-di-neutron* state of the alpha particle, and the *di-electron-di-proton-di-neutron* state of the helium atom. More complex coherent states, whether bosonic or fermionic, may also arise, and it is proposed that such states may be responsible for the shell structures of more massive elements, as observed in nature. In particular, it is claimed that this may be the driving force behind hybridization itself.

This paper is primarily concerned with three main things:

The first is a closer look at the spin-interaction geometries of degenerate electrons in a hybridized atomic shell, those resulting in the lower energy states described in Hund’s Second Rule. This occurs first in the cases of boron and carbon.

The second is a conjecture about how *di-electron* orbitals might affect unpaired electron orbitals within the same shell, by causing them to become constricted laterally, and therefore somewhat extended, radially. Such an orbital extension would take with it the electron’s properties of charge, field, and spin.

The third is a conjecture about the form of hybridization that occurs in the *d*-block transition elements, namely *pd*-hybridization. It is proposed that this hybridization involves only

the  $p$ - and  $d$ -orbital electrons, allowing optimal symmetries to form *without* the need to include the  $3s^2$  *di-electron*. That *di-electron* can then remain as a type of ‘fundamental’ resonance for the 3<sup>rd</sup> shell, within which (or upon which) the  $pd$ -hybrid orbitals resonate as superimposed harmonics. Such an  $s$ -orbital resonance may in fact serve to stabilize and symmetrize the 3<sup>rd</sup> shell structure as a whole into a coherent quantum wave structure.

It is proposed that the electron geometries that result from this consideration of  $pd$ -hybridization may help to explain the physical mechanisms behind several observed chemical and magnetic properties in atomic and metallic systems, not least among them, the paramagnetic strength trend across the periodic table. It is further proposed that, along with the concept of orbital constriction and extension mentioned above, these  $pd$ -hybrid geometries may help to explain the mechanism of the iron atom’s strong ferromagnetism.

## 2. SUB-QUANTUM ORBITALS

This approach differs from traditional approaches in that orbitals are conceptualized through a different paradigm — the absolute relativistic sub-quantum mechanics developed by Williamson and van der Mark [1,2,3], and reflected in the related mathematical framework according to the Williamson equation. This equation,  $\mathcal{D}_\mu \Xi_\nu = 0$ , employs a Clifford-Dirac algebra in order to represent an absolute relativistic set of coupled linear differential equations that allow each aspect of a quantum system’s energy to be identified discretely in wave function modeling [2].

While spherical harmonics are successful in describing the electron distribution within the hydrogen atom, it does not work as successfully in multi-electron systems. This is because electrons interact with one another on multiple levels — charge, field, and spin. Further, their spin interactions appear to occur in three separate phase relationships: the intrinsic photon angular momentum, the rotating photon topology’s angular momentum in an orthogonal direction, and the overall tumbling structure in the second orthogonal direction [4]. These aspects of spin exist in a perfect phase-locked harmony in the ratio  $\hbar : \frac{1}{2}\hbar : \hbar$ .

As such, a new approach is sought that combines electrons in symmetrical, phase-locked stationary wave structures, and that also takes into account the interactions between their charges, fields, and spins that will seek their lowest energy interaction state.

It is not possible to imagine such lower energy states if the nature of the interactions themselves are not understood, conceptually, at the sub-quantum level. As such, the sub-quantum mechanics approach [2] opens a window into the subatomic particle realm that was previously inaccessible.

All stable quantum structures must be resonant, coherent, quantized, harmonic systems. This is because, at their core, they are photon wave topologies. Stationary waves have structural elements that appear to remain stationary, even as energy is flowing continuously and symmetrically throughout the system. So too it must be with electrons in orbitals. They are not so much orbiting but rather inhabiting a shared wave topology in perfect phase with one another...

indistinguishable from one another when they are degenerate. Together, they constitute a single atomic quantum state. It is therefore not useful to think of the electrons in an interacting state by comparing them to that same multiple of non-interacting electron states. These states are simply of a different nature.

Within an atomic shell, it is proposed that electron interactions will be dominated by whether the electrons are unpaired, unpaired while spin-bonding [4], or in the paired *di-electron* state [3]. It is proposed — and seems self-evident — that: a spin-bonding electron will require higher ionization energy to remove than an unstabilized unpaired electron; an electron from a *di-electron* resonance will require an even higher ionization energy to remove; an electron from a full shell resonance will require the most ionization energy. At first glance, that appears consistent with the ionization energy trend across the periodic table [9], though this is not conclusive of anything on its own.

It is well known that *di-electron* orbitals repel more strongly than unpaired electron orbitals. This concept will be applied in describing possible electron orbital symmetries that result from hybridization in the second row and transition metal elements. However, specific wave function modeling of each will be left for future work.

### 3. $sp^2$ -HYBRIDIZATION

#### 3.1: Hybridization

Boron (B) has an electron configuration of  $1s^2 2s^2 2p^1$ . With five electrons, it is the first atom to contain electrons that are in a *p*-orbital. This is not a sphere-shaped harmonic in a single-electron hydrogen atom, and so a single electron in a *p*-orbital cannot find a symmetrical arrangement around a sphere by itself.

Boron therefore cannot simply add its *p*-electron into the same ( $2s^2$ ) configuration that beryllium (Be) has, as imagined in figure 1 (*below, right*), because it would not be stable. If an electron spent half of its wavelength in one lobe and half in the opposite lobe, ‘zittering’ back and forth across the atom, it would also not be stable. Stable electron waves require a spherical, in-phase, and ‘stationary’ symmetry.

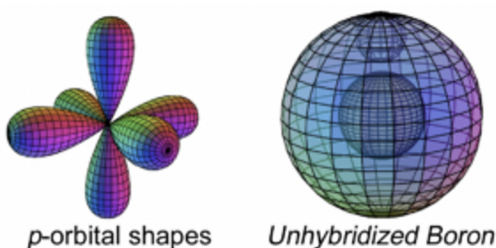


Fig. 1: The *p*-orbital lobes (*left*).



The asymmetry of boron's 5th electron therefore causes the two paired electrons in the  $2s$  orbital to uncouple from their *di-electron* state in order to form a fermionic *tri-electron* state with the single  $p$ -electron. This not only allows all three electrons to equilibrate their energy, but also puts these identical, indistinguishable electrons into a single resonant harmonic wave. An  $sp^2$ -hybridization results. While, for two of the three electrons, this represents an increase in energy, the collective state compensates by allowing for an energy-lowering that is much more significant.

Although it may be convenient to think of this as involving the  $s$ -orbital and two of the three  $p$ -orbitals of the 2<sup>nd</sup> shell, it is, in fact, three new equal-energy (degenerate) orbitals. They allow the electrons to achieve maximum stability by assuming a triangular (trigonal planar) arrangement around the core electron shell. This minimizes repulsion by having the electrons as far from one another as they can get, as well as stabilizing all three into a coherent, spin-linked harmonic state through the energy lowering of Parallel Spin Bonding (PSB) [4].

### B: $1s^2 2s^2 2p^1$

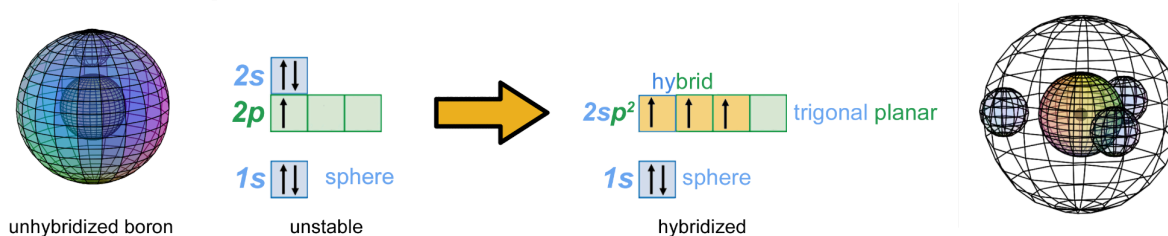


Fig. 2: The orbital diagram for boron. The large empty wireframe (above, right) indicates the boundary of the 2<sup>nd</sup> shell [7].

Note carefully that the small spheres within the 2<sup>nd</sup> shell in figure 2 (above, right) simply indicate the *directions* of maximum electron density. The actual orbital shapes will be more like three equal longitudinal sections of the shell or sphere (see fig. 3 below). We might imagine that each orbital occupies one third of the volume of the shell, though not uniformly, as electron density will have a maximum at the center of the orbital and will decrease towards the orbital boundary due to electron repulsion. But electron density will nonetheless fill the entire shell in order to shield the positive charge of the nucleus in every direction.

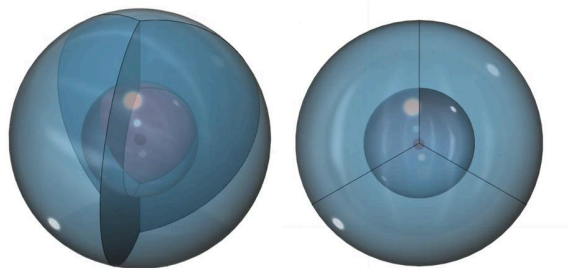
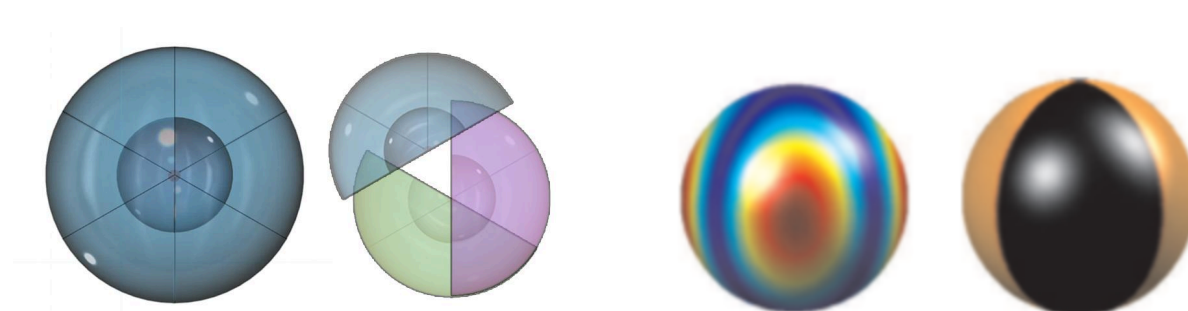


Fig. 3: The orbital diagram for boron, showing the three 2<sup>nd</sup> shell degenerate orbitals as equal longitudinal slices

We might equally well consider the spin-bonding unpaired electron orbitals to be overlapping in ‘spin space’ [3], as shown in figure 4 below. In such a case, each electron in the *tri-electron* state resonates through *half* of the shell’s volume at a time, while overlapping in the trigonal fashion depicted.

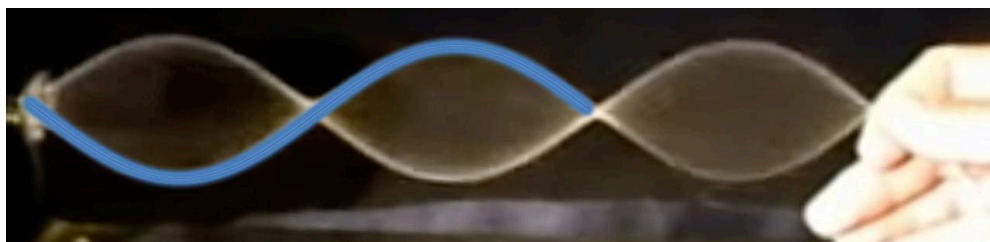


*Fig. 4: Boron’s three  $2sp^2$ -orbitals surrounding a  $1s^2$  core di-electron shell (top left), shown with overlapping sub-orbitals (top, right) [7], and as a spherical harmonic (bottom) in which the blue (or tan) color represents the non-zero nodes in the wave structure.*

In either case, each of the three hybrid orbitals contains one electron. Or more accurately: three unpaired same-spin electrons are resonating together into a single spherically-symmetrical stationary-wave harmonic resonance structure.

Whether or not the orbital symmetries are as clearly defined as depicted here, this geometry might serve as a first approximation when integrating the volume of spin phase overlap in order to represent spin bonding numerically. In that case, half of the 2<sup>nd</sup> shell’s volume will involve parallel spin-bonding (PSB) [3,4]; each of the three electrons will experience a one-third volume overlap with each of its adjacent electrons. We might therefore speculate that between one fourth and one half of the spin-space energy in the 2<sup>nd</sup> shell is reduced as a result of this resonance. This describes the essential mechanism of Hund’s Second Rule: the energy-lowering of angular momentum reduction that results from the energy sharing of spin-bonding.

It seems logical that the overlapping case (*in fig. 4*) might be a more accurate representation (*than in fig. 3*), simply because, when a stable stationary wave develops, each individual wave within the structure can be seen as being composed of two adjacent antinodal regions, which overlap with others in order to represent the complete structure (*see fig. 5 below*).



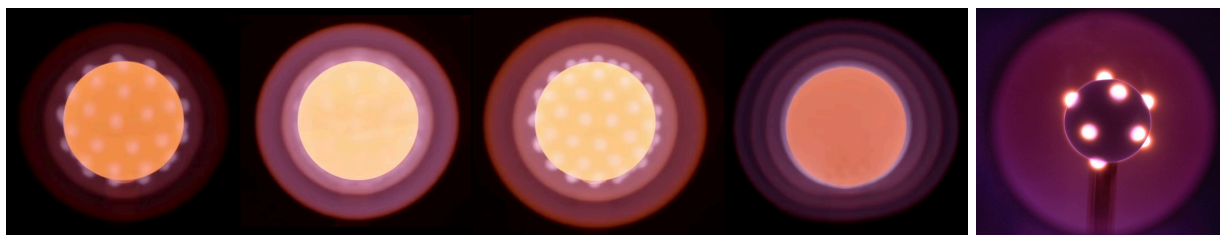
*Fig. 5: Overlapping wave (blue) within a stationary wave resonance.*

On the other hand, since the three antinodes (and their nodes) will be equally distributed around the atom, the non-overlapping view can be seen as a convenient way to divide the shell volume between its equivalent electronic components. What may be drawn as a clear boundary between sub-orbitals would then simply mark the *center* of the nodal boundary — through which energy is nonetheless continually flowing.

### 3.2: A Plasma Analogy

A useful analogy for visualizing atomic orbitals might therefore be to think of them almost as if they are plasma tufts around a spherical electrode.

One tool for visualizing such ‘tufts’ might be the images taken from the work of the SAFIRE Project [5]. During the operation of their reactor, various stable plasma states and concentric plasma shells have been generated and photographed around the spherical electrode, as shown below. These structures appear to be separated by nodal regions of low though non-zero electron density, or perhaps akin to Langmuir electric double layers. What is more, the distribution of small tufts around the electrode appears to evoke a platonic-style regular spherical symmetry. That should not be surprising, given the symmetry and maximized repulsion distance required by electron domains in an atomic or molecular system.



*Fig. 6: Several examples of plasma tufts and shells from the SAFIRE Project [5], generated around the spherical electrode in their reactor.*

The comparison between the plasma tufts and shells of an electrode and atomic orbitals is invoked, not simply because of the visual similarity that might be imagined, but because electromagnetic plasma phenomena are known to be scalable [6].

The analogy to the atom might go further still. An atom might be thought of as behaving in a similar manner to an electrode, in terms of its charge interactions — a positive nuclear ‘anode’ surrounded by a negatively charged virtual cathode that is the harmonic electron wave constituting the orbitals. One could even imagine considering the single atom as a sort of continuous ‘plasma,’ since it is made up of a coherence between positive and negative fermions, and produces orbital regions that may be similar to an electrode plasma sheath.

Further, while the electrodes pictured above represent a macroscopic system, and their tufts (and shells) will each contain a large number of electrons at this scale, if such a plasma were scaled down to the size of a single atom, it is conceivable that the tufts could be composed of either one electron or a *di-electron*, since these are the units of quantization in atomic orbitals.

The image on the far right in figure 6 above, for example, might evoke the concept of a valence shell with 12 electron domains.

#### 4. $sp^3$ -HYBRIDIZATION & OCTET EXPANSION

Although  $sp^3$ -hybridization is a familiar concept in chemistry, the orbital structures of carbon (C), neon (Ne) and argon (Ar) will be considered in order to underscore the differences between the present approach and the traditional approach.

##### 4.1: Carbon (C)

Carbon (C) has an electron configuration of  $1s^2 2s^2 2p^2$ . In this case, the  $sp^3$ -hybridization that occurs allows the atom to achieve tetrahedral symmetry involving the  $s$ -orbital and three  $p$ -orbitals of the 2<sup>nd</sup> shell. Like boron, carbon cannot simply add its two  $p$ -electrons into the same ( $2s^2$ ) configuration that beryllium (Be) has because it would not be stable. The asymmetry therefore causes the two paired electrons in the  $2s$  orbital to uncouple from their *di-electron* state in order to form a fermionic *tetra-electron* state with the two  $p$ -electrons.

The four equal-energy (degenerate) electrons can now achieve maximum stability by assuming a 4-directional (tetrahedral,  $sp^3$ -hybridized) arrangement around the core electron shell. This minimizes repulsion by having their regions of maximum electron density as far from one another as they can get.

##### C: $1s^2 2s^2 2p^2$

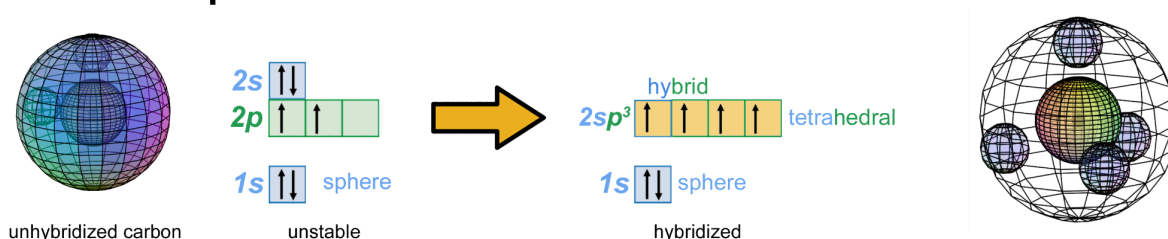


Fig. 7: The orbital diagram for carbon. The large wireframe (top, right) indicates the boundary of the 2<sup>nd</sup> shell.

Note again that the small spheres within the 2<sup>nd</sup> shell in the image above simply indicate the *directions* of maximum electron density. The orbitals themselves will be more like four equal tetrahedral sections of the shell, or a 4-lobed tetrahedral wave (*see fig. 8 below*). Each orbital occupies one fourth of the volume of the shell, though not uniformly, as electron density has a maximum at the center of the orbital and decreases towards the orbital boundaries due to electron repulsion. But electron density will nonetheless fill the entire shell in order to shield the positive charge of the nucleus in every direction. In the carbon atom, each of the four hybrid orbitals contains one electron.

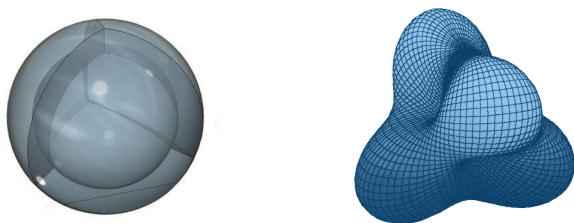


Fig. 8: Four  $sp^3$  orbital lobes (left) [7] and tetrahedral spherical harmonic wave (right).

As in the case of boron, though, we might equally well consider the spin-bonding unpaired electron orbitals to be overlapping in ‘spin space’ (see fig. 9 below). In this case,  $5/12^{\text{th}}$  [8] of the  $2^{\text{nd}}$  shell’s volume will involve parallel spin bonding (PSB), as each electron experiences a volume overlap (region A in fig. 9) with each of its three adjacent electrons.



Fig. 9: Overlapping shell segments of the  $3^{\text{rd}}$  spherical harmonic ‘note’ [8].

Four-directional (tetrahedral) symmetry is significant because, after the sphere, it is the first multi-directional symmetry that can attain near perfect spherical symmetry. While the three-directional ( $sp^2$ ) symmetry of boron is symmetrical in the equatorial direction, it is not spherically symmetrical since its axial electron density will be lower than its equatorial electron density.

It is possible that electron spin in these tetrahedral sub-orbitals will be radially oriented (in the absence of an external magnetic field), since this allows for greatest symmetry, and therefore, degeneracy. If so, carbon’s  $2^{\text{nd}}$  electron shell would be a spin-zero region that is nowhere not spinning.

Note that carbon does not exist in nature in its isolated atomic form, being always bonded to at least one other atom. That does not render this discussion merely theoretical, however, because, in order to measure ionization energy, elements are atomized in gaseous form before being ionized. In such cases, atoms will adopt their most symmetrical electron structures, both before and after ionization. The first ionization energy of carbon should therefore represent the removal of one electron from this spin-bonding, *tetra-electron* resonance structure. That should be more difficult than removing one from the *tri-electron* resonance structure in boron, which it is [9].

## 4.2: Trans-Carbon Asymmetry

In the case of nitrogen, oxygen, and fluorine, however, their  $sp^3$ -hybridization will not be perfectly symmetrical. Nitrogen’s 4 electron domain directions contain 3 unpaired electrons and



one *di-electron* (pair) in a tetrahedral arrangement. *Di-electrons* contain greater electron density than a single electron, they are diamagnetic, and they therefore repel more strongly than an unpaired electron. ‘Lone pairs’ consequently take up more volume than unpaired electrons in the orbital wave resonance, as is well known in traditional chemistry.

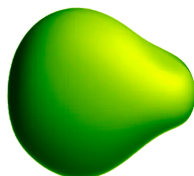
We therefore expect that nitrogen’s three degenerate unpaired 2<sup>nd</sup>-shell electrons will collectively occupy a little less than three fourths of the shell volume.

Since oxygen’s  $sp^3$ -hybridization contains two *di-electron* pairs and two unpaired electrons, the *di-electrons* will occupy a little more than half of the shell volume, with the two unpaired electrons forced to share the volume that remains. (This is the reason that the H-O-H bond angle in the water molecule is  $104.5^\circ$  rather than a perfectly tetrahedral  $109.5^\circ$ .)

### 4.3: Fluorine: Orbital Constriction & Extension

Fluorine’s  $sp^3$ -hybridization contains *three di-electrons* and only a *single* unpaired electron. This last unpaired electron will therefore occupy much less than one fourth of the shell’s volume because it will experience *constriction* as a result of the strong repulsion it feels from *all three* of the *di-electrons* surrounding it.

It is here proposed that this will cause this unpaired electron orbital to be extended radially outward in response to this lateral constriction. (It will be limited in the extent to which it can be compressed inward, due to the outward repulsion and electron density of the inner shell *di-electron* beneath it.) Fluorine’s unpaired electron orbital may therefore bulge outward, beyond the average radius of the three *di-electron* hybrid orbitals, resulting in an innately asymmetrical atom. (This is depicted in an exaggerated manner in figure 10 below.)



*Fig. 10: fluorine’s bulging unpaired electron orbital resulting from di-electron constriction*

If this conjecture is correct, it may be this ‘bulging’ unpaired electron orbital — in addition to the high effective nuclear charge and great desire for a full shell resonance — that contributes to fluorine’s extreme reactivity. This reactivity can also be seen as a statement about the full-shell configuration of neon — about the large amount of energy that is released when it is adopted. It is so stable because it is a highly symmetrical and bosonic quantum electron state (see §4.4).

This concept of orbital constriction and outward extension may also find application further up the periodic table, when we consider the hybrid orbitals of the transition metals. Specifically, it may play an important role in iron’s strong ferromagnetic character. (See §5.2.)

#### 4.4: Neon (Ne) & Argon (Ar)

In the case of neon (Ne), at the end of the second row of the periodic table, there is a full valence shell containing 8 electrons.

While carbon, nitrogen, oxygen, and fluorine all experience  $sp^3$ -hybridization, the traditional view of neon's full second shell involves a spherical  $2s^2$  orbital *di-electron*, with 6 unpaired *p*-electrons resonating within it in three mutually orthogonal directions.

It is here proposed, however, that the most stable, symmetrical, lowest energy state for the neon atom is achieved with 4 *di-electrons* in  $sp^3$ -hybridized tetrahedral symmetry. The 8 electrons sharing the small second (valence) shell would achieve lowest energy if they paired up, since both magnetic field and spin cancellation are maximized in *di-electron* formation [3]. With 4 *di-electrons* in tetrahedral symmetry, electron repulsion is minimized and the greatest distance between regions of maximum electron density can be maintained.

A comparison between the traditional approach and such a proposed structure is shown in figure 11 below.

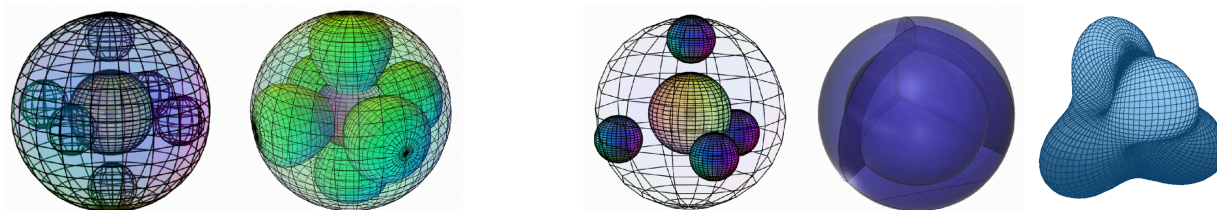


Fig. 11: The unhybridized version of neon's orbitals (left) with its traditional lobe view (green), compared to 3 representations of neon's tetrahedral *di-electron* orbital symmetry (right).

Another possibility is that the outer shell of neon constitutes an *octa-electron* spin-zero boson. This would have even more symmetry than the 4 *di-electron* case, and would allow for a greater degree of indistinguishability between the electrons of the single resonant harmonic system. Though it may not represent the lowest energy state of the system.

If the above proposal for neon is correct, the electron configuration of argon (Ar) should produce two nested spherical tetrahedra, aligned antiparallel (and anti-prismatic), as shown in figure 12 below.

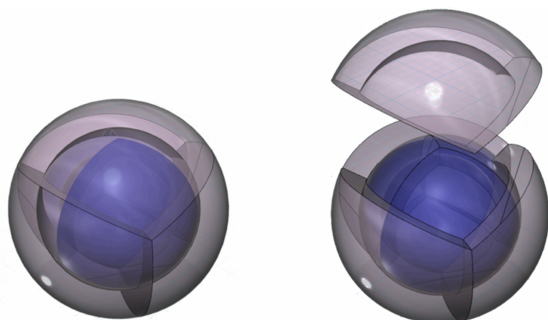


Fig. 12: Argon's nested tetrahedral orbital geometry (left), and with one outer orbital raised (right) for ease of viewing [7].

The reason that such a nested antiparallel tetrahedral geometry would be most stable is that the region of lowest electron density on one shell would be aligned opposite the region of highest electron density on the shell above or below, thereby minimizing repulsion between shells. In the diagram above, the vertex where the nodes *between* orbitals intersect would be a point of lowest electron density. It lies directly opposite the center of the face of the orbital above or below it, which is the point of highest electron density in that orbital. Such an overlap would therefore represent the lowest energy state.

While the entire atom can freely rotate, the two shells should maintain their relative orientation by way of holding the atom in its preferred, lowest energy state.

#### 4.5: Sulfur's Expanded Hybridization

In the case of neon above, we suggested that 6 unpaired *p*-orbital electrons, arranged in 3 orthogonal directions, would not be stable, yet that is the structure of the sulfur atom when its octet is fully expanded.

Like oxygen, the sulfur (S) atom contains 6 valence electrons, with two *di-electrons* and two unpaired electrons found in a tetrahedral  $sp^3$ -hybridized arrangement. When a sulfur atom is approached by highly electronegative atoms, such as oxygen or fluorine, their high electronegativities can induce one or both of sulfur's valence *di-electrons* to uncouple, yielding up to 6 unpaired electrons available for bonding, in up to six-directional  $sp^3d^2$ -hybridization.

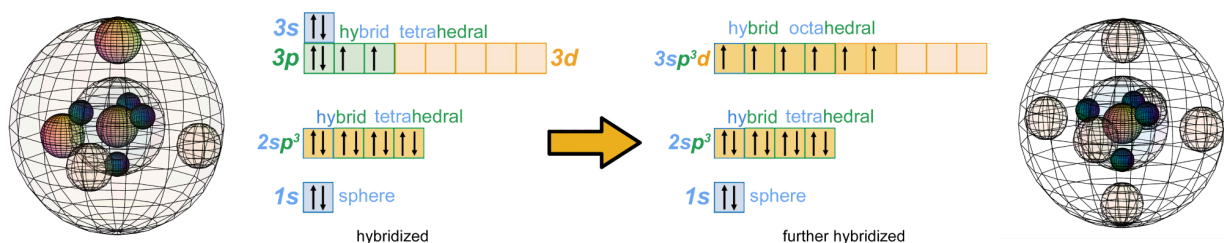
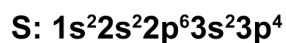


Fig. 13: Orbital diagrams for sulfur hybridizing into an octahedral  $sp^3d^2$ -hybridized geometry

The sulfur hexafluoride ( $SF_6$ ) molecule's 6 covalent bonds in octahedral symmetry<sup>1</sup> is an example of this structure. This is possible for sulfur but not oxygen because sulfur's outer 3<sup>rd</sup> shell contains a larger volume than oxygen's outer 2<sup>nd</sup> shell. It can therefore accommodate more electron density — in the case of  $SF_6$ , the presence of 12 electrons.

While this octahedral symmetry (fig. 13, on the right) looks just like the geometry of the traditional *p*-orbitals shown earlier (in fig. 1), it is important to note that it is *not* made up of just *p*-orbitals. It is a hybridization that combines 3*s*-, 3*p*-, and 3*d*-orbitals. Further, it only occurs

<sup>1</sup> Octahedral, because its 6 bonding sites define the vertices of an 8-faceted volume.



when induced into this state by highly electronegative bonded atoms attracting its electron density *outwards*.

This geometry will not manifest, though, when a single sulfur atom is ionized. The first ionization energy of sulfur should therefore represent the removal of one of the electrons from one of its two *di-electron* sub-orbitals in  $sp^3$ -hybridization. (It will not come from one of the unpaired electrons. The reason for this is discussed in §6 below.)

In fact, if the structure proposed above for neon is correct, it would mean that there is no case in nature where  $p$ -orbitals exist in three mutually orthogonal directions, as they are modeled in traditional quantum mechanics for the single-electron hydrogen atom. When  $p$ -orbitals are present along with other orbitals in the same space, they must always hybridize because mutual electron interactions at close-range, in the same atomic shell, cannot be avoided.

## 5. $pd$ -HYBRIDIZATION

It is here proposed that when  $p$ - and  $d$ -electrons occupy the same shell, their interactions invite us to consider them as a hybridized unit rather than as independent, superimposed harmonic structures. Even so, there will still remain energetic differences between orbitals within a hybridization as a result of geometric and electron interaction asymmetries. (This is analogous to energy differences between the *di-electron* and single electron orbitals within the  $sp^3$  hybridization of, say, oxygen.)

As illustrated in figure 14 below, one  $s$ -orbital coupled with the three  $p$ -orbitals yields up to 4-directional ( $sp^3$ -hybridized) symmetry for up to 8 electrons. Three  $p$ -orbitals coupled with five  $d$ -orbitals yields up to 8-directional symmetry for up to 16 electrons.

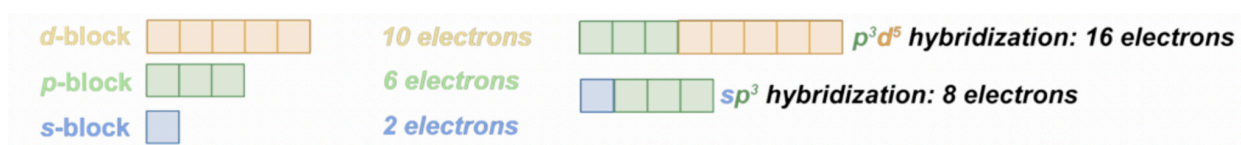


Fig. 14:  $pd$ -hybridization

Using the traditional nomenclature as our guide, we will call these  $p^3d$  (tetrahedral) through  $p^3d^5$  (hexagonal bipyramidal or cubic) symmetries. The resulting 4-, 5-, 6-, and 8-directional symmetries are shown in the diagram below for the  $3d$  transition metals. The asymmetry of a 7-directional geometry means that the electron wave state will find a way to avoid it, if possible.

Note carefully again that, in the diagrams below, the small spheres are only intended to show the relative *directions* of the electron domains, *not* their shape. (The lightly colored wireframe spheres represent unpaired electrons and the full color spheres represent *di-electrons*.)

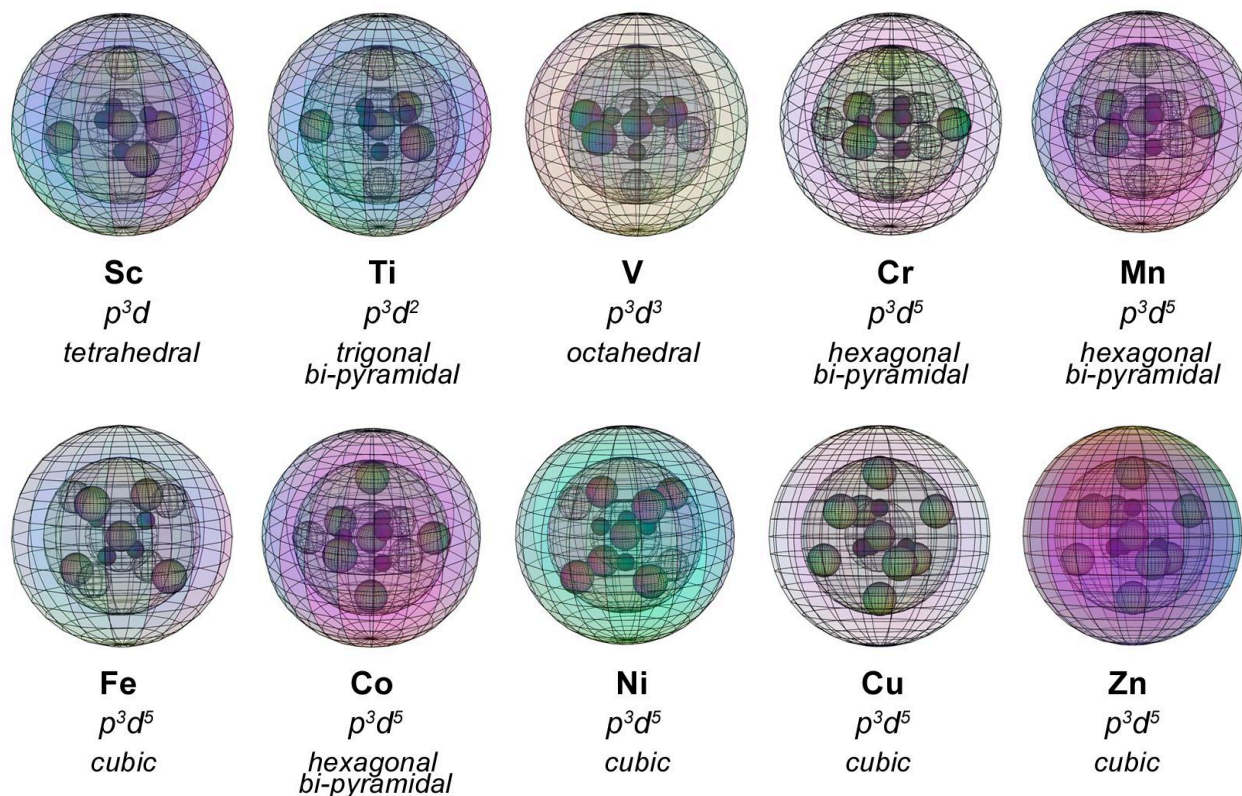


Fig. 15: *pd*-hybridization and electron domain geometries for the 3d transition metals [7].

In 3<sup>rd</sup>-shell *pd*-hybridization, the 3s-orbital electrons are not needed in order to achieve stable symmetry. A 4s-electron is nevertheless available to help the hybrid orbitals achieve optimal symmetry, if needed. This is known to occur in several cases, for example chromium (Cr) and copper (Cu). (Chromium, for example, would be stuck with an asymmetrical 7-directional electron geometry in its 3<sup>rd</sup> shell if an electron from the 4s-orbital did not drop down into the 3<sup>rd</sup> shell to help it achieve a much more stable 8-directional symmetry.)

This persisting 3<sup>rd</sup>-shell *di*-electron (see fig. 16 below) does introduce a form of wave resonance that has not occurred on previous elements. There now remains a spherical *di*-electron, within which the *pd*-hybrid orbital electrons resonances can be supported and stabilized. Even when the 4s valence electrons are delocalized during (metallic) bonding, the core electron geometry will remain the same, still stabilized by the persisting 3<sup>rd</sup>-shell *di*-electron.

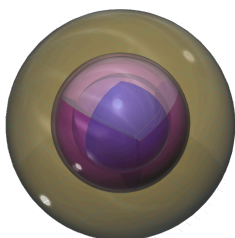


Fig. 16: Alternative view of the orbitals of scandium (see §5.1. below) showing the persisting 3s<sup>2</sup> *di*-electron around its core shell.

It would be expected that such a new form of resonance would manifest as a chemical property change, and in fact, this is the point on the periodic table where the transition metals show up. They have properties that are quite distinct from previous elements.

Within such  $pd$ -hybrid orbitals, if  $di$ -electrons and unpaired electrons occupy the same shell, the larger  $di$ -electron repulsion will predominate, determining the base geometry because they repel more strongly. As we saw in the case of nitrogen, oxygen, and fluorine above, this is simply because  $di$ -electrons contain twice the electric charge of single electrons, they are diamagnetic, and they occupy more volume as a result of their higher electron density and greater repulsion. Single, unpaired electron repulsion will therefore be satisfied secondarily, filling in the remaining electron domain directions in the most symmetrical fashion possible.

While the electron and  $di$ -electron symmetries might not be identical in  $pd$ -hybridization, they must still each attain (stationary wave) symmetry in order to be stable. Overall symmetry might therefore not be perfectly platonic, but it will be the best “2-way” symmetry attainable for the system, just as we saw with boron’s (trigonal planar) 2-way symmetry.

In the case of titanium’s 5-directional symmetry (*see fig. 15 above*), it is proposed that the 3  $di$ -electrons will assume a trigonal planar arrangement in order to maximize distance and minimize repulsion, and the two unpaired electrons will be repelled into the two (furthest) axial positions, above and below that plane.

It is here proposed, and the details will be clarified in later work, that:

- These  $pd$ -hybridized electron geometries, and the interactions they bring to bear, appear to account for the trend in paramagnetic strength across the  $3d$  transition metals. (This trend does *not* go simply according to the number of unpaired electrons present.)
- One of the two proposed factors that facilitates ferromagnetism in iron (Fe), cobalt (Co), and nickel (Ni) results from electron interactions between specific  $pd$ -hybridized geometries within the crystalline metallic structure.

Observational evidence that might support the present proposal regarding transition metals electron domain geometry can be seen in positron annihilation radiation spectroscopy (2D-ACAR) images of copper’s Fermi surface.

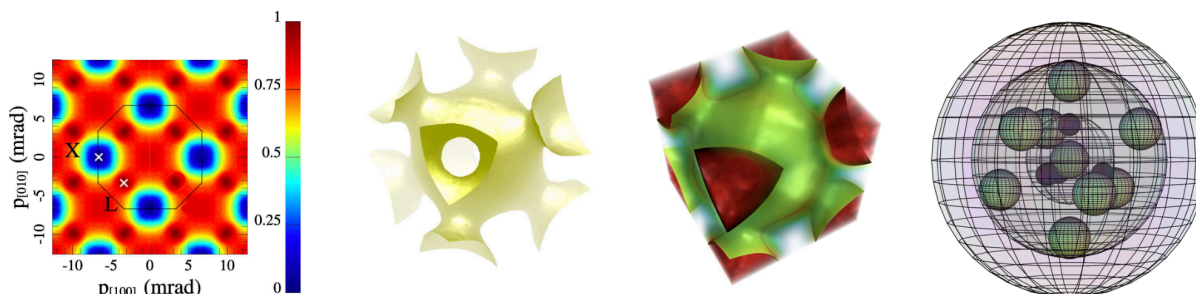


Fig. 17: Fermi surface in copper, imaged via 2D-ACAR spectroscopy [11], along with proposed structure for Cu (far right)

## 5.1: Scandium (Sc)

Scandium ([Sc](#)) is the first element to feature a  $d$ -orbital electron. It is here proposed that a 4-directional symmetry can be achieved with  $p^3d$ -hybridization. This yields tetrahedral symmetry involving 3  $di$ -electrons and 1 unpaired electron *without* involving the  $3s$ -orbital electrons. The  $3s$ -electrons can therefore remain in their spherical  $di$ -electron state, *within which* (or perhaps *upon which*) the other  $3^{\text{rd}}$  shell electrons resonate, stabilized, like harmonics upon a fundamental.

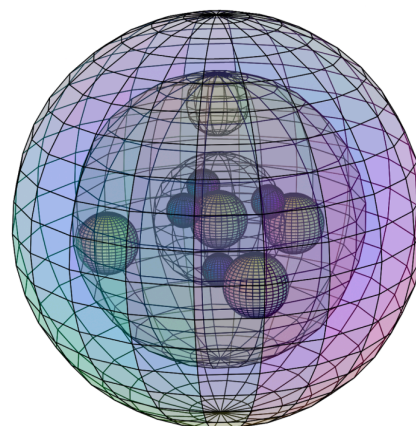
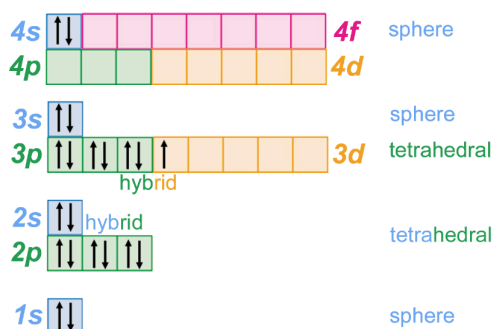
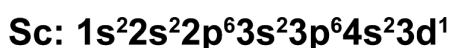


Fig. 18: The orbital diagram for  $p^3d$ -hybridized scandium (Sc) [7]

As seen in figure 18, the  $3^{\text{rd}}$ -shell tetrahedral symmetry will also align both antiparallel and antiprismatic to the  $2^{\text{nd}}$  shell tetrahedral  $di$ -electrons within it, in order to minimize mutual  $di$ -electron repulsion. The  $4s^2$  valence  $di$ -electron shell surrounds the atom, or is delocalized during metallic bonding. As such, this atom's spectrum should reflect three different signatures for the  $3^{\text{rd}}$  shell electrons, i.e. the  $3s^2$   $di$ -electron, the three  $3p^3d$   $di$ -electrons, and the single unpaired  $3p^3d$  electron.

## 5.2: Iron (Fe)

Iron is the sixth element with electrons in the  $d$ -orbital, and it has a uniquely symmetrical electron structure among the  $3d$  transition metals.<sup>2</sup>

It is proposed that iron has a  $3^{\text{rd}}$  shell containing 4  $di$ -electrons and 4 unpaired electrons in  $p^3d^5$ -hybridized cubic symmetry, all resonating within a spherical  $3s^2$  orbital. The 4  $di$ -electrons and 4 unpaired electrons will arrange themselves in a highly symmetrical, alternating fashion that minimizes repulsion. This electron domain geometry (*shown in fig. 19 below*) can arguably more correctly be viewed as two intersecting, antiparallel (and anti-prismatic) tetrahedral structures, one containing  $di$ -electrons, the other single electrons.

<sup>2</sup> Even though nickel, copper, and zinc also have a cubic electron domain geometry, they do not have the added symmetry of iron's alternative electron- $di$ -electron orbital structure.



In such a configuration, the 4 tetrahedral *di-electrons* in the 2<sup>nd</sup> shell will be aligned directly beneath the unpaired electrons in the 3<sup>rd</sup> shell in order to minimize inter-shell repulsion with the *di-electrons* in the 3<sup>rd</sup> shell.

It is here proposed that it is this unique and highly symmetrical structure of unpaired core electrons that gives iron its important magnetic properties. (The details of iron's ferromagnetic mechanism will be explored in future work.)

### Fe: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$

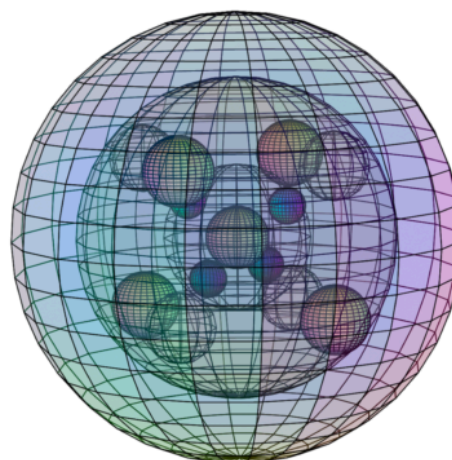
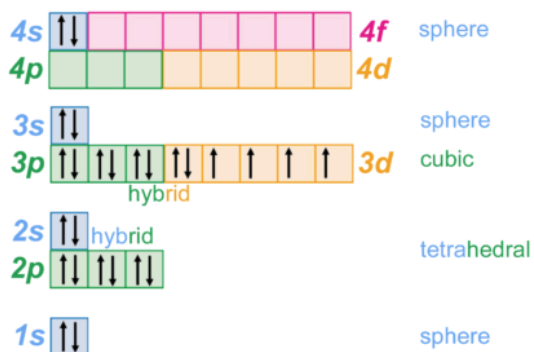


Fig. 19: The orbital diagram for  $p^3d^5$ -hybridized iron (Fe) [7]

Iron's 3<sup>rd</sup> shell antiparallel double tetrahedral symmetry is also known as a dual tetrahedron, in which each point also coincides with a corner of a cubic structure. Interestingly, when an iron crystal is magnetized, it adopts a body-centered cubic lattice, which is the same electron geometry as double-tetrahedral, just viewed from a different angle, as shown below.

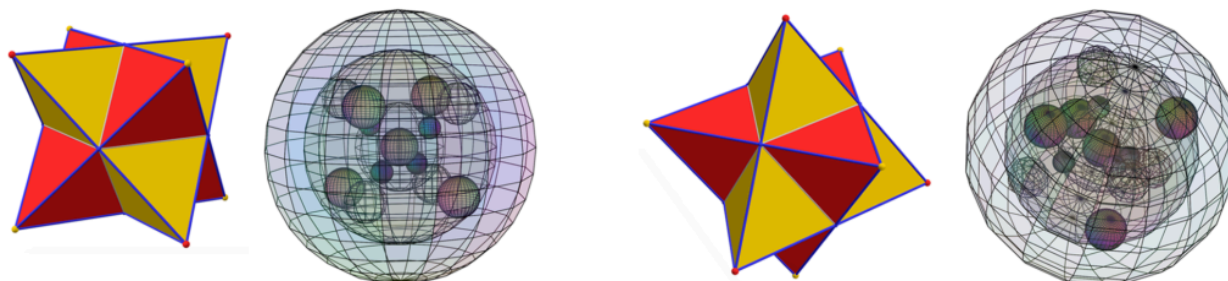


Fig. 20: 'Cubic' and 'tetrahedral' views of an iron atom along with a dual tetrahedron formed from two 'antiparallel' intersecting tetrahedra.

It is proposed that the great symmetry and stability of this double-tetrahedral structure is one of the two factors contributing to iron being the most strongly ferromagnetic element. The other has to do with a slightly different form of inter-shell and inter-atom orbital spin interaction within the crystal, one similar to that proposed above for fluorine. (See §5.3.)

### 5.3: Ferromagnetic Spin-Bonding

In the geometry of iron proposed above, the four unpaired electron orbitals are all surrounded by (four) same-shell *di-electrons*. They will therefore all be laterally constricted, in the same way that we proposed above for the fluorine atom. In addition, each unpaired electron orbital in iron's 3<sup>rd</sup> shell has an inner-shell *di-electron* orbital immediately beneath it. That adds even more repulsion and constriction from *below*.

Since the valence electrons in a metal crystal are delocalized by way of metallic bonding, [10] iron's eight  $p^3d^5$ -hybrid orbitals appear on the surface of the atomic cores within the crystal, resonating upon and stabilized by the 'fundamental' that is the  $3s^2$ -*di-electron*. The four tetrahedrally-arranged unpaired electron orbitals are also extended radially outward, into the crystalline interatomic distances between the atomic cores, as a result of the amount of constriction and extension they experience from the *di-electrons* beside and beneath them.

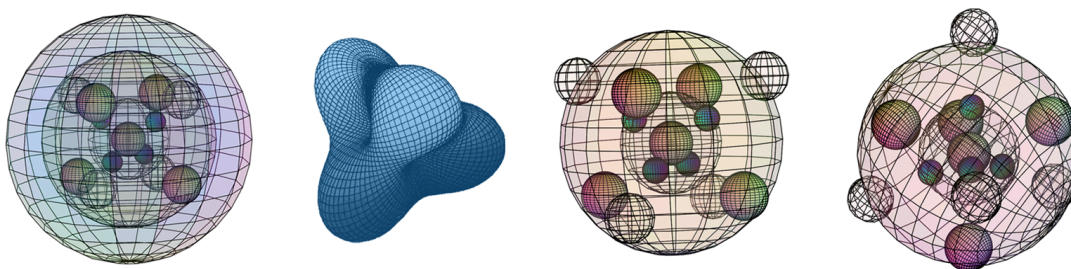


Fig. 21: 'Cubic' geometry of an iron atom (left) along with three views of its unpaired electron orbital extension due to constriction.

It is proposed that, in a crystal, this brings the electrons on adjacent iron atom cores into a range across which inter-atomic electron interactions become more significant. This form of crystal interaction is here dubbed 'ferromagnetic spin-bonding,' and it will be further detailed in future work, along with investigating why iron, cobalt, and nickel are the *only* transition metals to be naturally ferromagnetic, even though their periodic table neighbors, chromium and manganese, have *more* unpaired electrons. It will also be investigated how this model appears to account for the trends in relative melting points versus Curie Temperatures for these three ferromagnetic metals, as well as their hard versus easy crystal directions of magnetization.

## 6. *d*-BLOCK ION GEOMETRY

When in metallic form, the valence *s*-orbital electrons of a metal become delocalized, and when in 2+ ionic form<sup>3</sup>, they are removed. In both cases, the inner electron geometry should remain the same.

It is here proposed, however, that when the 3+ ion forms, an electron is removed from one of the core *pd*-hybrid *di-electrons*, and *not* from one of the unpaired electrons or from the  $3s$

<sup>3</sup> Or the 1+ form in the case of chromium or copper (in the 3*d* row).

orbital *di-electron*. This occurs in order to achieve the most symmetrical electron structure. If it were to lose an unpaired *pd*-hybrid electron, the symmetry would be reduced from 8- to 7-directional, which would then simply force one of the *di-electrons* to dissociate in order to reconstitute 8-directional symmetry. If it were lost from the 3*s* *di-electron*, the fundamental would be weakened for all of the other hybrid electrons, representing a less stable overall state.

In the cobalt (Co) atom, the 3<sup>rd</sup>-shell hybrid orbitals contain 5 *di-electrons* and 3 unpaired electrons, to yield 8-directional symmetry. The loss of two 4*s*-electrons to form the Co<sup>2+</sup> ion will still retain that 3<sup>rd</sup>-shell (hexagonal bipyramidal) geometry. If a third unpaired electron is then lost to form the Co<sup>3+</sup> ion, there will remain 5 *di-electrons* and 2 unpaired electrons, yielding 7-directional geometry with no 4*s*-electrons left to redeem its symmetry. The loss of an electron from one of the *di-electrons*, however, will yield 4 *di-electrons* and 4 unpaired electrons, for an 8-directional cubic (or ‘double-tetrahedral’) 3<sup>rd</sup> shell geometry. This is a far more stable and symmetrical configuration, and the same one that is here proposed for the iron (Fe) atom, the element before cobalt on the periodic table.

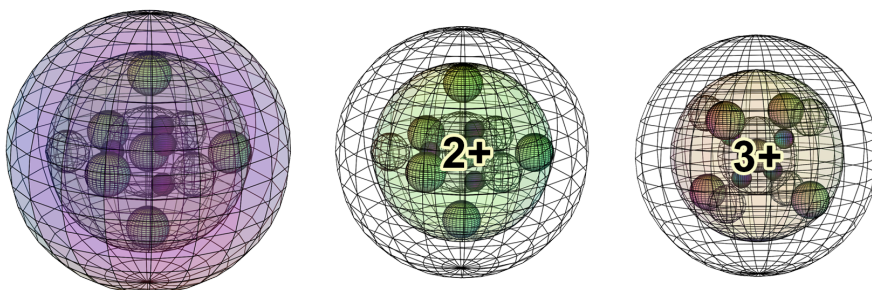


Fig. 22: The orbitals of cobalt (left), the Co<sup>2+</sup> ion (center), and the Co<sup>3+</sup> ion (right)

## 7. CONCLUSION & FUTURE WORK

The primary conclusions of this paper are:

- Spin-mediated electron interactions (also known as ‘spin-bonding’) help determine atomic orbital and hybridization geometries within atomic electron shells.
- The stronger repulsion of many *di-electrons* can cause the constriction and radial extension of adjacent unpaired electron orbitals within a shell.
- It is proposed that this process occurs in fluorine’s valence shell, and that it may contribute, along with the several other known factors, to its very high reactivity.
- It is proposed that *pd*-hybridization occurs in the electron shells of the transition metal atoms, stabilized upon an *s*-orbital *di-electron* foundation, yielding 8-directional geometries that would otherwise not be considered without such a hybridization.
- It is proposed that, in the case of iron, it is the combination of its *pd*-hybrid geometry — a remarkably symmetrical cubic, double-tetrahedral 3<sup>rd</sup>-shell symmetry — along with the significant constriction and radial extension of its unpaired electron orbitals, that causes its strong ferromagnetism.

Future work will investigate and seek to model the consequences of these hybrid electron structures in more detail.<sup>4</sup> These will include:

- modeling how such electron and orbital interactions affect (or dictate) the values and trends in ionization energy and electron affinity,
- accounting for the strength trend in *d*-block paramagnetism, based upon *pd*-hybridization,
- investigating the mechanism of ferromagnetism in more detail, including why *only* iron, cobalt, and nickel are ferromagnetic in the *d*-block,
- Investigating antiferromagnetism in more detail, including proposing that chromium's antiferromagnetism is not a form of ferromagnetism, but rather an 'electron-gas' coupling.
- introducing *pdf*-hybridization and possible ground-state electron geometries for neodymium (Nd) and gadolinium (Gd) that help to account for their magnetic properties.

## 8. ACKNOWLEDGEMENTS:

This approach, that we like to call sub-quantum chemistry, is based upon and is made possible by advances in the fields of relativistic quantum mechanics achieved by JGW in collaboration with Martin B. van der Mark, and in nuclear physics with Vivian N.E. Robinson. Their friendship, consultation, and mentorship have been invaluable in the process of developing this work.

The authors would like to thank Brian J. Drouin, Innes Anderson-Morrison, Mayank Drolia, and Michael Rudolph for valuable discussions regarding this material.

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<sup>4</sup> Appropriate software tools are currently under development at the Quantum Bicycle Society ([www.Quicycle.com](http://www.Quicycle.com))



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