CORRESPONDENCES BETWEEN THE CLASSICAL THOMSON PROBLEM AND THE PERIODIC TABLE OF ELEMENTS

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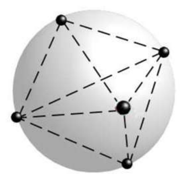
Thomson Problem

Distribution of N equal point charges (e.g. electrons, protons) on a unit sphere having a global minimum electrostatic Coulomb interaction energy

$$U(N)=\sum_{i<j}^{N}\frac{1}{|r_i-r_j|}$$

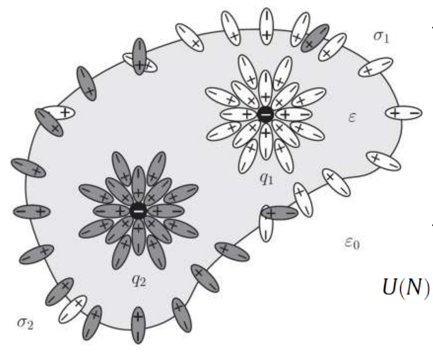


A natural result of J.J. Thomson's classical "plum pudding" model of the atom[1] without a uniform, positively-charged spherical background.

The general mathematical solution of the Thomson Problem remains UNKNOWN.[2]

An interactive database of Thomson Problem solutions is hosted by *Syracuse University*.[3]

Discrete Charge Dielectric (DCD) Model[5]



Types of electrostatic interactions among discrete charges in a dielectric:

Coulomb Repulsion among point charges: $q_1 \leftrightarrow q_2$

Direct Polarization among point charges and charges they polarize directly: $q_1 \leftrightarrow \sigma_1$, $q_2 \leftrightarrow \sigma_2$

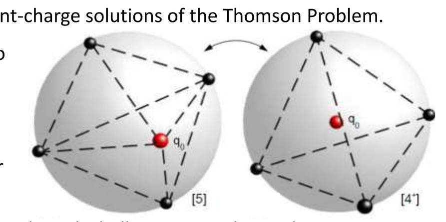
Indirect Polarization among point charges and charges polarized by other electrons $q_1 \leftrightarrow \sigma_2$, $q_2 \leftrightarrow \sigma_1$

The total energy stored in a dielectric object with N free charges is

$$U(N)=\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}U_C(q_i,q_j)+\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}U_{ind}(q_i,q_j)+\sum_{i=1}^{N}U_{dir}(q_i,\sigma_i)$$

Discrete Configuration Changes in the Thomson Problem

Consider energy difference between configurations of neighboring N point-charge solutions of the Thomson Problem.



Moving one charge, q_0, to the origin allows the remaining N-1 charges to form an N-1 configuration.

The distribution of energies associated with this configuration change (open circles in plot at right) exhibits a few abrupt jumps and dips that correspond with remarkable fidelity to electron shell-filling behavior found throughout the periodic table! (See Additional Reading)

Lower energies coincide with electron shell closures; higher energies coincide with shell openings. Changed in point charge configurations in the Thomson Problem correspond to changes in orbital (single electron wavefunction) shapes.

Point Groups, the Thomson Problem, and the Periodic Law

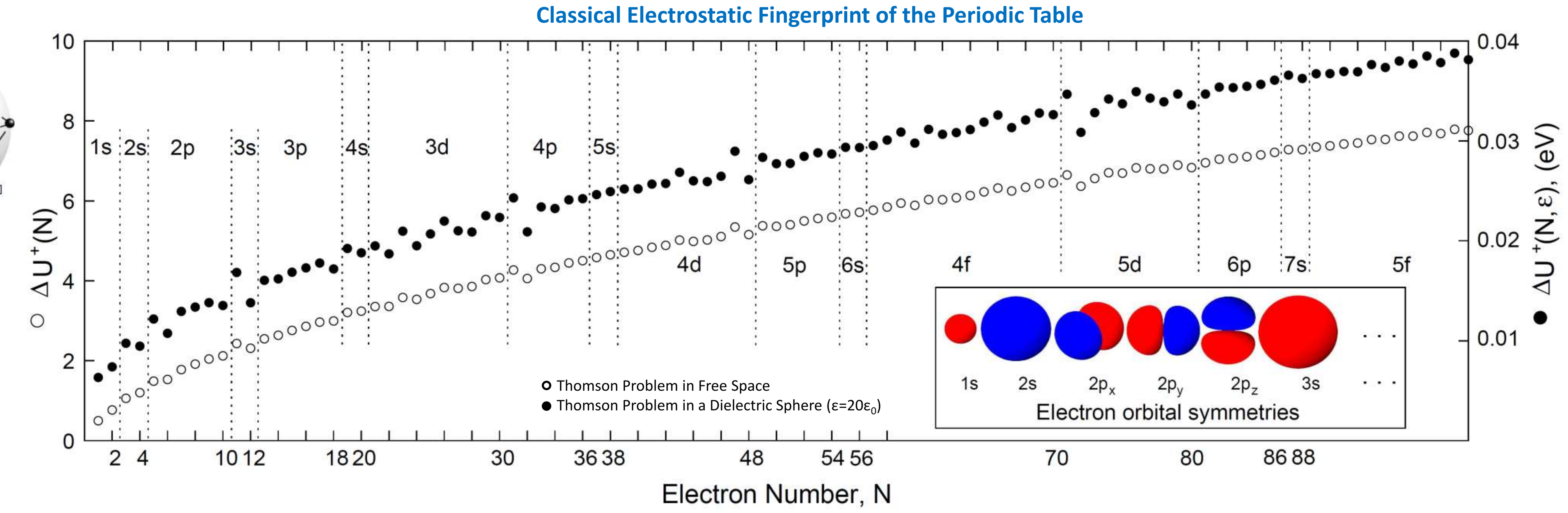
The most salient features appear at N = (11,12), (31,32), (47,48) and (71,72).

These large energy drops are regularly/periodically distributed in the range $1 \le N \le 100$ and have highly symmetric point groups known as I_h, T_d, O, and I, respectively. Note: This spacing regularity is not found in solutions of the Thomson Problem for $N > 100$ (see below). Conjecture: The periodic table is special because atoms have few (<100) electrons.

Notably, each of these highly symmetric solutions of the Thomson Problem have very similar, low-symmetry point group neighbors: N = 11, 13 both have C_{2v} point groups. N = 31, 33 have C_{3v} and C_s point groups, respectively. N = 47, 49 both have C_3 point groups. N = 71, 73 both have C_2 point groups. These neighboring symmetries may be observed in the periodic table below showing the energy of each electron in every solution of the Thomson Problem ($1 \le N \le 101$).

These four salient features are consistent with the distribution of *empirical size-normalized ionization energies*. (below)

Classical Electrostatic Fingerprint of the Periodic Table



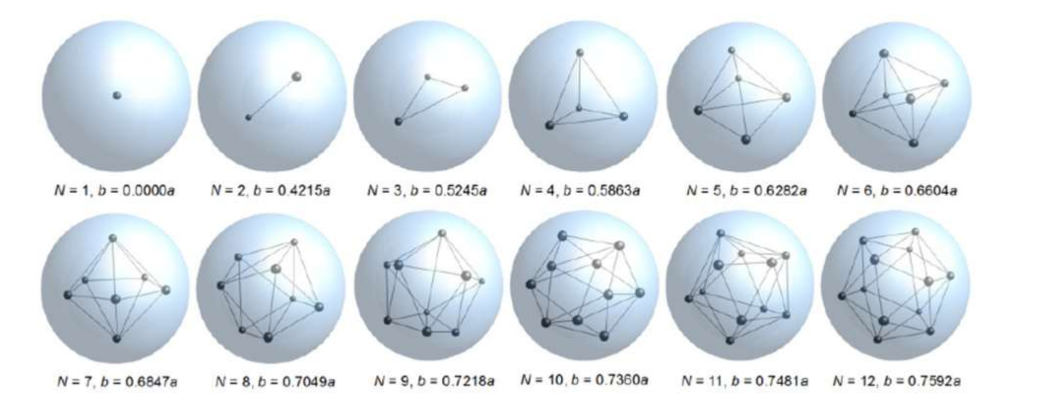
Thomson Problem in a Dielectric Sphere

Spherical quantum dots are also known as "artificial atoms" because many shell-filling phenomena appear in their quantum mechanical treatments, or "designer atoms" as their electronic properties may be tailored for device purposes.

In this work, a quantum dot is treated using the **classical** Discrete Charge Dielectric model as a dielectric sphere of radius a, assuming solutions of the Thomson Problem for free charges in the sphere. The "Thomson sphere" has radius $b < a$).

As electrons are added to the dielectric sphere, the size of the Thomson sphere increases.

Variation of the Thomson radius, b, results in more pronounced features in the Classical Electrostatic Fingerprint of the Periodic Table (shown at left) when treated within a dielectric sphere compared to a fixed unit sphere in free space.[6]



Charge Hardness of the Thomson Problem

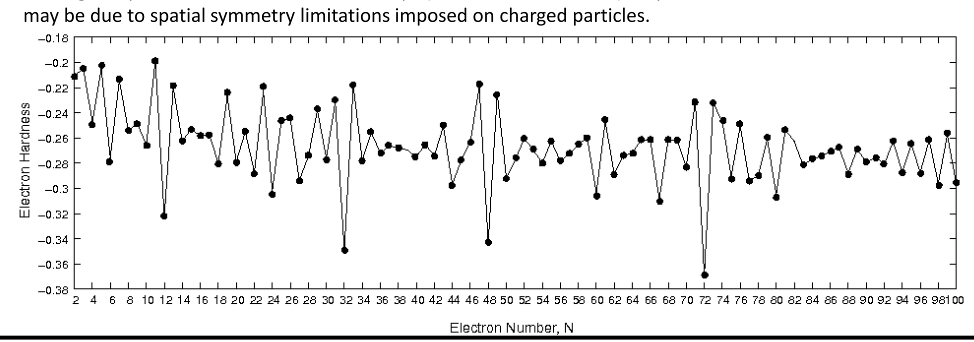
Charge hardness is the difference between the ionization and affinity energy of a single charge,

$$\eta = I - A = |U(N)-U(N-1)| - |U(N)-U(N+1)|$$

The principle of "hardness" is central to the hard-soft acid-base (HSAB) model in Chemistry.

Charge hardness of the Thomson Problem reveals several features that may be related to atomic and nuclear structure:

1. An even/odd trend (lower even-N / higher odd-N) suggests that even-N solutions are higher in symmetry than odd-N, and that there is an energetic preference for "paired" charges – indicative of Pauli's exclusion principle.
2. Reversal of even/odd trend between $24 < N < 29$ may correspond to half-filled, low-lying 4s shells in chromium (Z = 24) and copper (Z = 29) – known shell-filling rule violations. (cf. electron configurations in periodic table below.)
3. The "string" of hardness values between $83 \le N \le 87$ indicates similar preferences for the addition or removal of a single charge. Notably, bismuth (Z = 83) has the largest known stable nucleus. (A connection to nuclear structure.)
4. The regular, periodic occurrence of salient dips (N = 12, 32, 48, and 72) may be indicative of the Periodic Law which may be due to spatial symmetry limitations imposed on charged particles.



Periodic Table of Electron Energies in the Thomson Problem

Electrostatic energy associated with each electron in solutions of the Thomson Problem is collected in the shape of a periodic table below. Several patterns and correspondences with natural atoms are observed.

Octet Rule

In Chemistry, the "Octet Rule" is a rule of thumb stating that configurations of eight valence electrons are obtained when atoms chemically combine. In most models valence electrons occupy an outermost shell. The Thomson Problem, however, has only one "shell" since all electrons reside on a unit sphere. Despite this, the Octet Rule is observed!

The Octet Rule is primarily applied to atoms having few electrons (N < 20). For larger atoms, the rule is less stringent.

The 18th column on the periodic table (inert or noble gases) includes very stable elements.

For N = 10, there are 8 electrons in one energy level of the Thomson Problem, and 2 in another. These are consistent with the conventional shell-filling rules: fill the $1s^2$ orbital and then the $(2s^2 + 2p^6)$ valence shell – the 1st and 2nd rows of the Periodic Table (or "periods"). (cf. periodic table below.)

Similarly, for N = 18, the $1s^2$ shell is filled, followed by 8 electrons in the $(2s^2 + 2p^6)$ shell, then 8 in the $(3s^2 + 3p^6)$ valence shell – the first three "periods" of the Periodic Table.

Unlike other models that require three distinct electron shells to obtain three unique energy levels, the Thomson problem exhibits three energy levels within just one electron shell. This suggests that the Octet Rule is partly due to spatial symmetry/geometry properties associated with the Thomson Problem. This was not previously known.

Oxidation States

In the periodic table below, for sodium (Z = 11) and potassium (Z = 19) the Thomson Problem yields a single electron in the highest energy level. Sodium and potassium are well known to commonly exist in singly-ionized states (Na^+ and K^+).

After losing an electron, the new N-1 configurations are those of N = 10 and N = 18, respectively – the Octet Rule. The oxidation states of the first N = 20 systems are shown above the periodic table below.

Periodic Law

Consider the very stable inert/noble elements, krypton, xenon and radon and corresponding data in the table below.

A high degree of symmetry exhibited by electron occupancy of energy levels is observed in the Thomson Problem:

- For N = 36, there are 9 energy levels occupied by 4 electrons each.
- For N = 54, there are 27 energy levels occupied by 2 electrons each.
- For N = *86*, there are 43 energy levels occupied by 2 electrons each.

Energy level occupancy symmetry may be responsible for the Periodic Law. The physical nature of the Periodic Law is not (yet) understood! The present work may offer new insight.

Pauli's Exclusion Principle

Pauli's Exclusion Principle allows only two electrons to occupy the same energy level. An even number of electrons occupies most energy levels throughout solutions of the Thomson Problem. Moreover, the Thomson Problem exhibits a preponderance of paired electron energies.

Pauli's Exclusion Principle may be explainable in terms of charge pair symmetries in solutions of the Thomson problem.

Nuclear Phenomena

The phenomenon of charged pairs also applies to protons (e.g. alpha particles). Note that many plots below for N > 80 have charge pairs in their uppermost energy level.

Beta decay results in the gain/loss of a charge from the nucleus. Can you "map" any known decay chains through the data (e.g. the thorium, neptunium, or uranium decay chains) using the periodic table below and the charge hardness data to the left? Consider half-lives, net charge changes, etc.

One approach to include neutrons may be to consider them as part of the dielectric function of the model which *must* change during particle emission. Alpha particles, for example, have two protons and two neutrons.

Spatial Symmetry/Geometry Limitations

Discrete charges in 3-dimensional space are limited in the number of ways they can minimize their global energy. For example, consider that while 2, 3, and 4 charges can all be equidistant from each other, 5 charges can never all be equidistant. (Similarly, in 2-dimensions, like a sheet of paper, you cannot draw 4 equidistant points. Try it!) This symmetry/geometry property is unavailable to all N > 4 charge systems. Notice that N = 5 coincides with the first occurrence of a dumbbell-shaped *p*-orbital after the spherical 1*s* and 2*s* orbitals.

There are only 5 possible highly symmetric Platonic Solids having 4, 6, 8, 12 and 20 vertices. Notice that Z = 20 is the largest nucleus with an equal number of neutrons and protons. Larger stable nuclei have more neutrons than protons. The symmetry/geometry property found in the Platonic Solids is not found for more than 20-charge systems. Look it up!

Is size important? Features in the plot exist for all sphere sizes! Is there really a size-dependent "quantum regime"?

Quantum Numbers

Each particle in a system may be characterized by four quantum numbers:

Principal: n (SIZE of an orbital) **Magnetic**: m_l (ORIENTATION of an orbital in space)
Angular: l (SHAPE of an orbital) **Spin**: m_s (identifies each electron in an orbital)

Since most energy levels in the Thomson Problem are occupied by an even number of charges, it may be possible to identify each charge in each pair as being associated with either +1/2 or -1/2 "*spin*" – one on either side of the origin.

The spatial orientation of each pair may be defined (magnetic quantum number).

Electrostatic interactions are governed by geometric/symmetry operations that yield the orientation of each pair. SHAPE is merely a collection of geometric/symmetry operations. These may yield *angular* quantum numbers.

The Thomson Problem is confined to a unit sphere – the size is fixed. Within a dielectric sphere, the Thomson sphere varies in size. However, this is an insufficient correlation for orbital sizes in atomic electronic structure. One approach may include mathematically-equivalent image charges that exist outside the dielectric to comprehend atomic sizes.

It may be possible to construct the entire set of quantum numbers from the classical Thomson Problem.

Comparison with Empirical Size-Normalized Ionization Energies

The Thomson Problem is restricted to a unit sphere. Atoms vary in size (which is difficult to measure!).

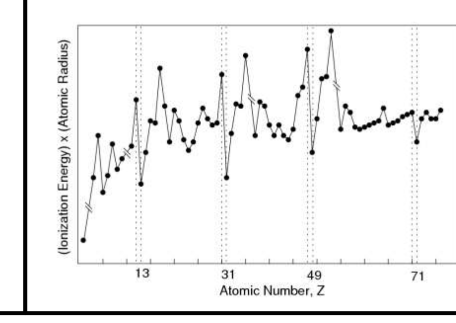
To compare the electrostatic energy distribution above to empirical quantities, the quantities must be normalized with respect to size. Empirical ionization energies[7] may be multiplied by empirical atomic radii[8] since energy is inversely proportional to size. Compare the plot below left with the plot above.

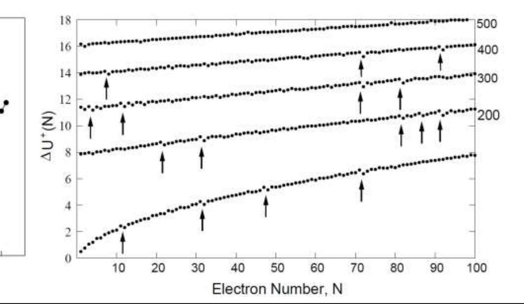
Two similarities are observed (See Additional Reading):

1. Energies increase in a similar manner as the number of electrons in the system increases.
2. The four largest energy dips in both distributions are in similar locations.

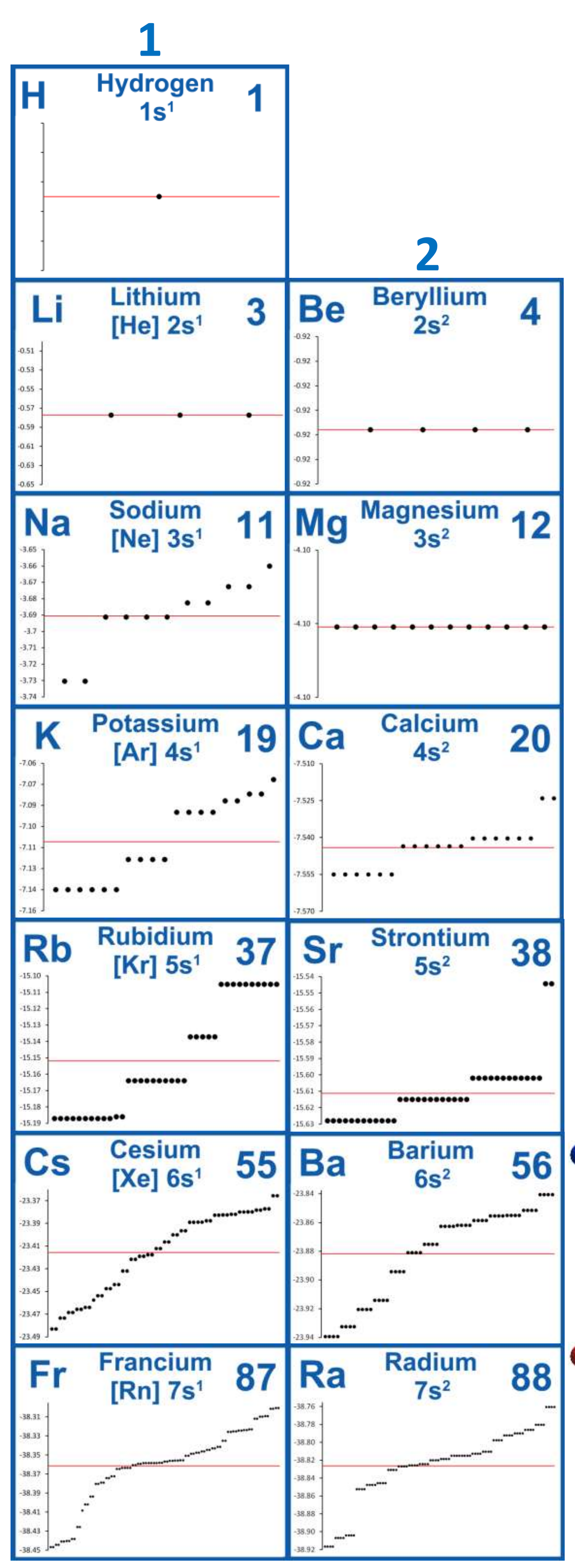
Hence, "fingerprint" is a good way to characterize the energy distribution above.

Additionally, since the four salient dips in energy appear with considerable regularity for $1 \le N \le 100$, they are evidence of the physical nature of the Periodic Law. It is curious that regularity of similar dips disappears for solutions of the Thomson problem for N > 100. (see below right).





Periodic Table of Electron Energies in the Thomson Problem



Notes

The electrostatic potential energy associated with each electron in solutions of the Thomson Problem are plotted in the form of the periodic table. The average energy per electron is shown as a **red** line.

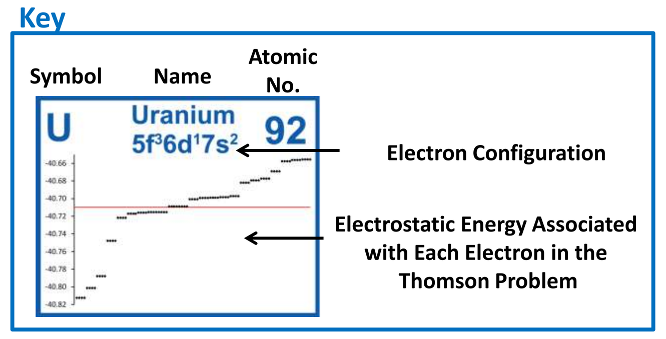
The electron configuration of each atomic system is shown for reference. For example, the shell-filling rule violation associated with chromium (Z = 24) may be identified as originating with the highly-symmetric 24-electron Thomson Problem configuration in which all 24 electrons have the same potential energy. Contrast this with energy level electron occupancy symmetries of neighboring systems.

Shell-filling rule violations are shown in **red**.

Energy levels appearing in the upper regions of each energy plot have the least negative potential energy. Use of the negative energy assumes that electrons reside in a negative potential well (though, strictly, the energies are positive given electron-electron interactions). They are plotted this way to indicate electrons that are least-bound to the system and therefore, the easiest to remove. As well, plotting them in this manner is potentially of a more useful, heuristic value for those familiar with band-structure theory in which "up" indicates "less bound".

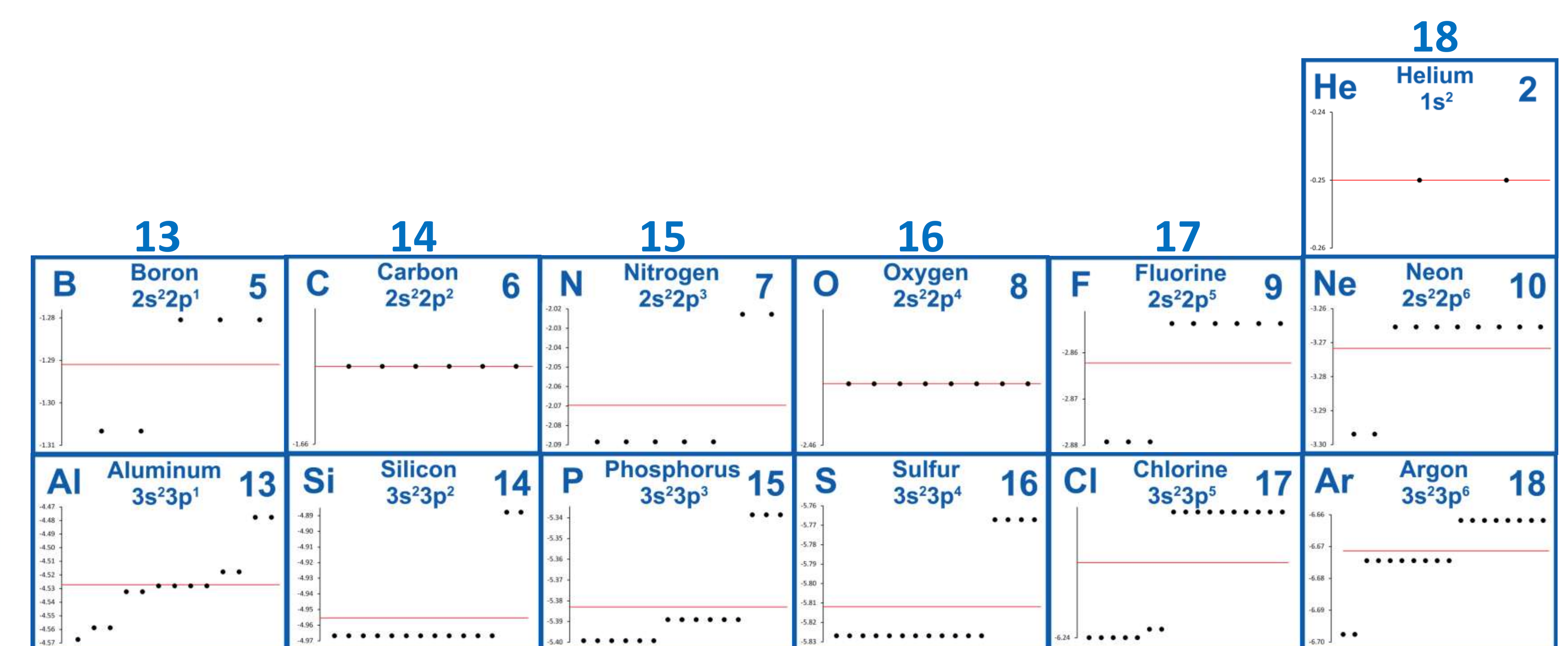
Several features of interest are described above. This is only a partial listing of correspondences between the Thomson Problem and atomic/nuclear structure. You're encouraged to explore this poster, identify new patterns and test them against known chemical and physical properties of atomic and nuclear structure. The Thomson Problem is *not* a complete description of atoms. There remains much work to be done.

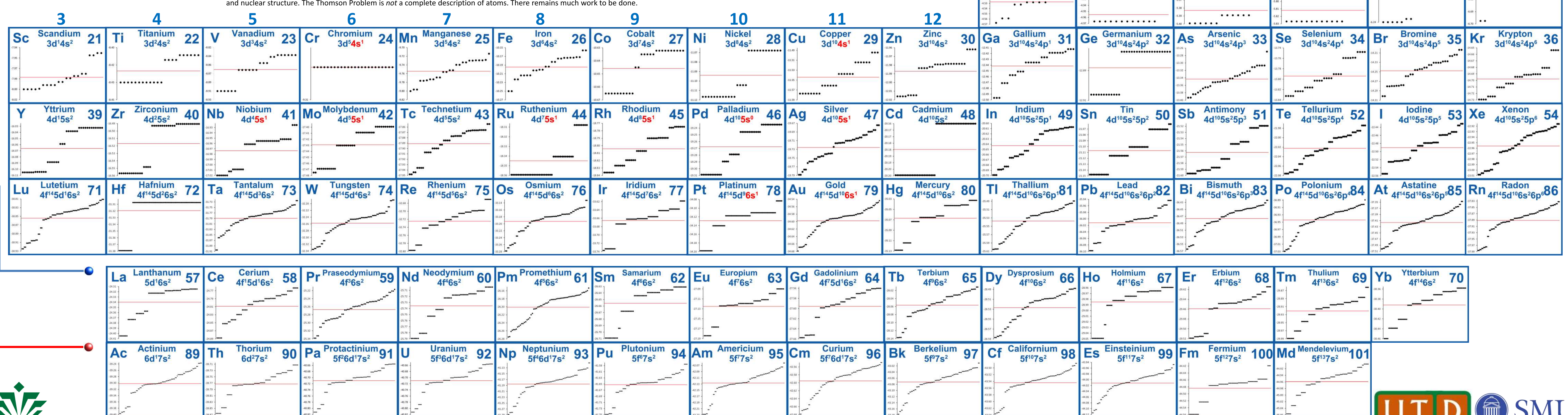
Key



Oxidation States

N:	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Electron Loss																	+7			
																+6	+6			
							+5								+5	+5	+5			
						+4	+4							+4	+4	+4	+4			
					+3	+3	+3						+3	+3	+3	+3	+3			+3
				+2	+2	+2	+2	+2				+2	+2	+2	+2	+2			+2	+2
	+1		+1	+1	+1	+1	+1	+1	+1		+1	+1	+1	+1	+1	+1	+1		+1	+1
Electron Gain	-1				-1	-1	-1	-1	-1		-1			-1	-1	-1	-1		-1	
						-2	-2	-2						-2	-2	-2				
						-3	-3							-3	-3					
						-4								-4						





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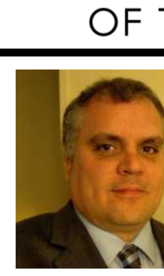

Bio Originally from the Weyauwega-Fremont school district of Wisconsin, Tim (TJ) LaFave Jr. holds doctoral (Electrical Engineering, 2006) and masters (Applied Physics, 2001) degrees from the *University of North Carolina, Charlotte*, and a bachelors degree (Physics, 1996) from the *Illinois Institute of Technology*, Chicago. In addition to this theoretical physics research in electrostatics, LaFave is interested in physics education research, and has more than a decade of experimental research experience including semiconductor and optoelectronic process engineering and device characterization. Results shown on this poster originated in his PhD dissertation[4] under the direction of Prof. Raphael Tsu as part of comparative classical and quantum mechanical studies on spherical quantum dots. Discovery of the "Classical Electrostatic Fingerprint of the Periodic Table" stems from his construction of the Discrete Charge Dielectric Model[5] of free electrons in the presence of dielectrics. Data plotted in the form of the Periodic Table were sorted in early 2013 to obtain a more-detailed comprehension of correspondences between the Thomson Problem and atomic and nuclear structure. LaFave maintains three search blogs accessible through pagesofmind.com.

Email tjlafave@yahoo.com | Twitter tjlafave | Facebook timlafavejr | ResearchGate Tim_LaFave_Jr | LinkedIn timlafavejr

References

[1] J. J. Thomson, *Phil. Mag.* **7**(39) 237-265 (1904).
[2] S. Smale, *Math. Intell.* **20** 7 (1998).
[3] Thomson Applet: http://thomson.phy.syr.edu/
[4] T. LaFave Jr. *The Classical Electrostatic Periodic Table, Capacitance of Few Electron Dielectric Spheres and a Novel Treatment of One- and Two-Electron Finite Quantum Wells* PhD dissertation, UNC-Charlotte, 2006. ONLINE: pagesofmind.com/TheChargedFew/1-0-the-original-thesis
[5] T. LaFave Jr., *J. Electrostatics*, **69** 414-418 (2011). arXiv:1203.3798v1
[6] R. Tsu & T. LaFave Jr. "Role of Symmetry in Conductance, Capacitance, and Doping of Quantum Dots" chapter appearing in *The Wonder of Nanotechnology*, M. Razeghi, L. Esaki & K. von Klitzing, eds., Ch. 1, (SPIE Press, 2013).
[7] Empirical Ionization Energies (NIST): http://physics.nist.gov/PhysRefData/IonEnergy/tblNew.html
[8] J. C. Slater, *J. Chem. Phys.* **41** (10) 3199–3205 (1964).

Additional Reading

T. LaFave Jr. "Correspondences between the classical electrostatic Thomson Problem and atomic electronic structure" *J. Electrostatics* 71(6) 1029-135 (2013).

T. LaFave Jr. "Discrete Transformations in the Thomson Problem" *J. Electrostatics* 72(1) 39-43 (2014).

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See pagesofmind.com/KeyToThePeriodicTable for a fresh approach to the Periodic Table based on this research.