Chemistry of the Super Heavy Elements

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Why Care?

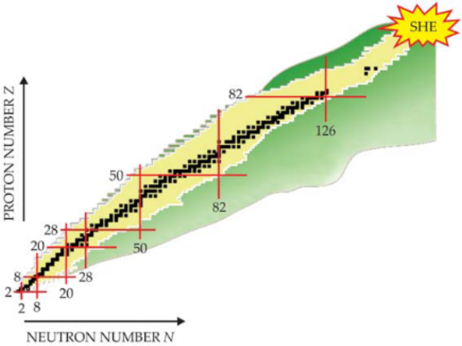

Figure: The Nuclear Landscape with the Super Heavy Elements (SHE). Figure from [3].

- "Island of stability" in the nuclear landscape near the SHE region [6]. What chemical properties do these exotic elements have?

Why the Island of Stability?

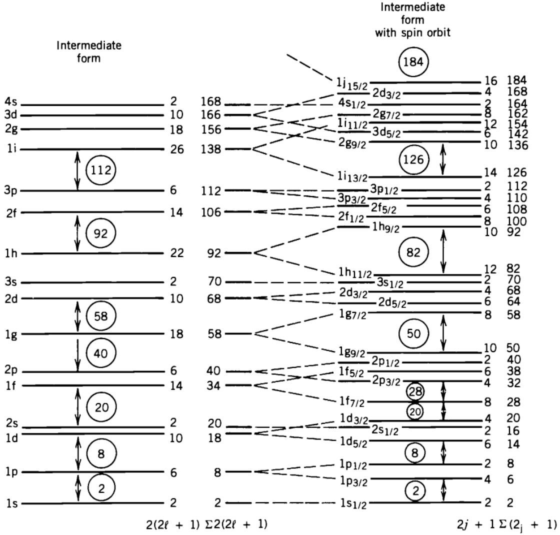

Figure: Enery levels in the Shell Model. Figure from Krane.

Shell Model

- Nucleon-Nucleon potential is given by Woods-Saxon:

$$V(r) = -\frac{V_0}{1 + \exp\left[\left(r - R\right)/a\right]}, \tag{1}$$

  plus a spin-orbit coupling.
- Filled nuclear shells, similar to filled atomic shells, are stable; called magic numbers.
- For instance, $^{208}_{82}\mathrm{Pb}$ is doubly magic and stable.
- $Z = 126$ and $N = 184$ expected to be stable.

Super Heavy Elements

- $Z \geq 104$ (Rf). Half-lives ranging from milliseconds to a few hours.
- Heaviest nuclei discovered is $Z = 118$ (Oganesson) by JINR, Dubna, Russia. Most stable isotope has $N = 176$.
- But how do we study them if they last only a few milliseconds? I'll answer this in my talk today.
- Before that, let's see what makes super heavy elements different.

Relativistic Effects

- For $Z \sim 100$, the Bohr velocity of electrons becomes relativistic.
- The energy levels using Dirac equation for hydrogen-like atoms are:

$$E_{n,k} = mc^2 \left(1 + \frac{Z^2\alpha^2}{\left(n - k + \sqrt{k^2 - Z^2\alpha^2}\right)^2} \right)^{-1/2} . \qquad (2)$$

- For $Z\alpha > 1$, the ground state energy becomes imaginary!
- Relativistic effects play a big role for SHEs.

Dirac-Coulomb-Breit Hamiltonian

- How do we deal with the relativistic problem?
- Numerically solve the many-body DCB Hamiltonian [4]:

$$H_{DCB} = \sum_i H_D(i) + \sum_{i<j} \left(\frac{1}{r_{ij}} + B_{ij} \right) \tag{3}$$

where,

$$H_D(i) = c\vec{\alpha}_i\vec{p}_i + c^2 (\beta_i - 1) + V^n(i), \tag{4}$$

and

$$B_{ij} = -\frac{1}{2} \left[\vec{\alpha}_i\vec{\alpha}_j r_{ij}^{-1} + (\vec{\alpha}_i\vec{r}_{ij}) (\vec{\alpha}_j\vec{r}_{ij}) r_{ij}^{-3} \right]. \tag{5}$$

- H_D is the Dirac Hamiltonian with external nuclear potential $V^n(i)$. The $1/r_{ij}$ is the Coulomb term and B_{ij} is the Breit-term coming from relativistic corrections.

Relativistic Stabilization

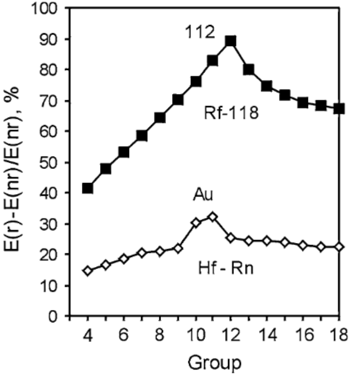

Figure: Relativistic stabilization of $6s$ and $7s$ shells. Figure from [4].

- Surprise: Simulations with relativistic calculations give higher stability to heavy elements.

Valence Shell Contraction

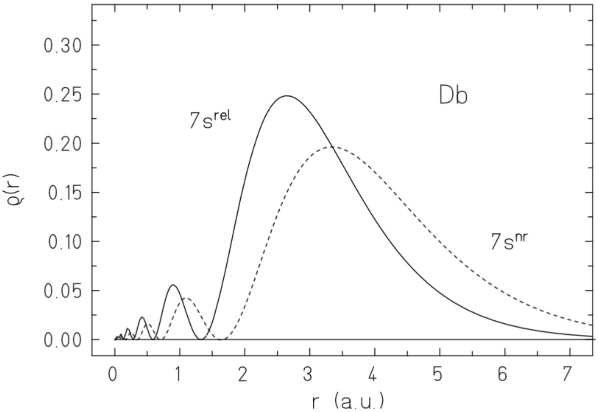

Figure: Relativistic (solid) and non-relativistic (dashed) radial distribution of the $7s$ valence electrons in Db ($Z = 105$). Figure from [4].

- Relativistic effects contract the valence shells! Chemically inert.

Fine Structure Splitting

IUPAC Periodic Table of the Elements

Key: atomic number
Symbol
name
abridged standard atomic weight

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 **H** hydrogen 1.0080 ± 0.0002																	2 **He** helium 4.0026 ± 0.0001
3 **Li** lithium 6.94 ± 0.06	4 **Be** beryllium 9.0122 ± 0.0001											5 **B** boron 10.81 ± 0.02	6 **C** carbon 12.011 ± 0.002	7 **N** nitrogen 14.007 ± 0.001	8 **O** oxygen 15.999 ± 0.001	9 **F** fluorine 18.998 ± 0.001	10 **Ne** neon 20.180 ± 0.001
11 **Na** sodium 22.990 ± 0.001	12 **Mg** magnesium 24.305 ± 0.002											13 **Al** aluminium 26.982 ± 0.001	14 **Si** silicon 28.085 ± 0.001	15 **P** phosphorus 30.974 ± 0.001	16 **S** sulfur 32.06 ± 0.02	17 **Cl** chlorine 35.45 ± 0.01	18 **Ar** argon 39.95 ± 0.16
19 **K** potassium 39.098 ± 0.001	20 **Ca** calcium 40.078 ± 0.004	21 **Sc** scandium 44.956 ± 0.001	22 **Ti** titanium 47.867 ± 0.001	23 **V** vanadium 50.942 ± 0.001	24 **Cr** chromium 51.996 ± 0.001	25 **Mn** manganese 54.938 ± 0.001	26 **Fe** iron 55.845 ± 0.002	27 **Co** cobalt 58.933 ± 0.001	28 **Ni** nickel 58.693 ± 0.001	29 **Cu** copper 63.546 ± 0.003	30 **Zn** zinc 65.38 ± 0.02	31 **Ga** gallium 69.723 ± 0.001	32 **Ge** germanium 72.630 ± 0.008	33 **As** arsenic 74.922 ± 0.001	34 **Se** selenium 78.971 ± 0.008	35 **Br** bromine 79.904 ± 0.003	36 **Kr** krypton 83.798 ± 0.002
37 **Rb** rubidium 85.468 ± 0.001	38 **Sr** strontium 87.62 ± 0.01	39 **Y** yttrium 88.906 ± 0.001	40 **Zr** zirconium 91.224 ± 0.002	41 **Nb** niobium 92.906 ± 0.001	42 **Mo** molybdenum 95.95 ± 0.01	43 **Tc** technetium [97]	44 **Ru** ruthenium 101.07 ± 0.02	45 **Rh** rhodium 102.91 ± 0.01	46 **Pd** palladium 106.42 ± 0.01	47 **Ag** silver 107.87 ± 0.01	48 **Cd** cadmium 112.41 ± 0.01	49 **In** indium 114.82 ± 0.01	50 **Sn** tin 118.71 ± 0.01	51 **Sb** antimony 121.76 ± 0.01	52 **Te** tellurium 127.60 ± 0.03	53 **I** iodine 126.90 ± 0.01	54 **Xe** xenon 131.29 ± 0.01
55 **Cs** caesium 132.91 ± 0.01	56 **Ba** barium 137.33 ± 0.01	57-71 lanthanoids	72 **Hf** hafnium 178.49 ± 0.01	73 **Ta** tantalum 180.95 ± 0.01	74 **W** tungsten 183.84 ± 0.01	75 **Re** rhenium 186.21 ± 0.01	76 **Os** osmium 190.23 ± 0.03	77 **Ir** iridium 192.22 ± 0.01	78 **Pt** platinum 195.08 ± 0.02	79 **Au** gold 196.97 ± 0.01	80 **Hg** mercury 200.59 ± 0.01	81 **Tl** thallium 204.38 ± 0.01	82 **Pb** lead 207.2 ± 1.1	83 **Bi** bismuth 208.98 ± 0.01	84 **Po** polonium [209]	85 **At** astatine [210]	86 **Rn** radon [222]
87 **Fr** francium [223]	88 **Ra** radium [226]	89-103 actinoids	104 **Rf** rutherfordium [267]	105 **Db** dubnium [268]	106 **Sg** seaborgium [269]	107 **Bh** bohrium [270]	108 **Hs** hassium [269]	109 **Mt** meitnerium [277]	110 **Ds** darmstadtium [281]	111 **Rg** roentgenium [282]	112 **Cn** copernicium [285]	113 **Nh** nihonium [286]	114 **Fl** flerovium [290]	115 **Mc** moscovium [290]	116 **Lv** livermorium [293]	117 **Ts** tennessine [294]	118 **Og** oganesson [294]

57 **La** lanthanum 138.91 ± 0.01	58 **Ce** cerium 140.12 ± 0.01	59 **Pr** praseodymium 140.91 ± 0.01	60 **Nd** neodymium 144.24 ± 0.01	61 **Pm** promethium [145]	62 **Sm** samarium 150.36 ± 0.02	63 **Eu** europium 151.96 ± 0.01	64 **Gd** gadolinium 157.25 ± 0.03	65 **Tb** terbium 158.93 ± 0.01	66 **Dy** dysprosium 162.50 ± 0.01	67 **Ho** holmium 164.93 ± 0.01	68 **Er** erbium 167.26 ± 0.01	69 **Tm** thulium 168.93 ± 0.01	70 **Yb** ytterbium 173.05 ± 0.02	71 **Lu** lutetium 174.97 ± 0.01
89 **Ac** actinium [227]	90 **Th** thorium 232.04 ± 0.01	91 **Pa** protactinium 231.04 ± 0.01	92 **U** uranium 238.03 ± 0.01	93 **Np** neptunium [237]	94 **Pu** plutonium [244]	95 **Am** americium [243]	96 **Cm** curium [247]	97 **Bk** berkelium [247]	98 **Cf** californium [251]	99 **Es** einsteinium [252]	100 **Fm** fermium [257]	101 **Md** mendelevium [258]	102 **No** nobelium [259]	103 **Lr** lawrencium [262]

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) APPLIED CHEMISTRY

- Recent numerical calculations predict an electron affinity of $0.076(4)$ eV [2] for Oganesson ($Z = 118$); a group 18 element.
- Flerovium, a group 14 element, is a closed shell atom with zero electron affinity [1].
- Fine-structure splitting of orbitals is responsible for these effects. A non-relativistic treatment will not predict them.

Real Experiments

- Although computer simulations are very powerful, what about real experiments?
- There are some results available for long-lived transactinides [5].
- I'm terrible at chemistry and don't want to embarass myself. But from what I understand, there are no discrepancies yet with computer calculations.

Summary

- Because of the short lifetimes involved, numerical simulation is the most powerful tool at our disposal.
- Relativistic effects result in some surprises.

Take-Home Message

- SHE research is exciting! Imagine how cool it would be to discover a stable SHE with exotic properties?

References

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