

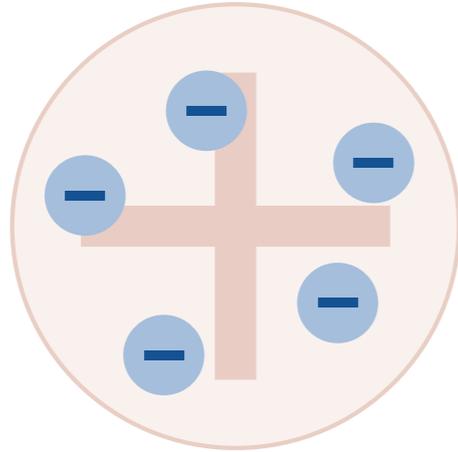
# Nuclear Structure and Isomerism

Ian Perry

MacMillan Group Literature Talk

April 29<sup>th</sup>, 2020

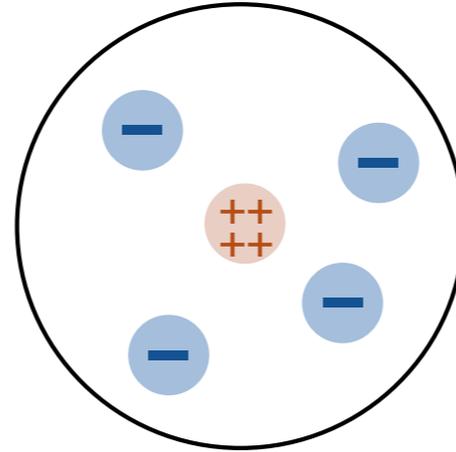
# History of Atomic Structure



**Thomson Model - 1904**

“Plum pudding” – A positive volume filled with negatively charged electrons.

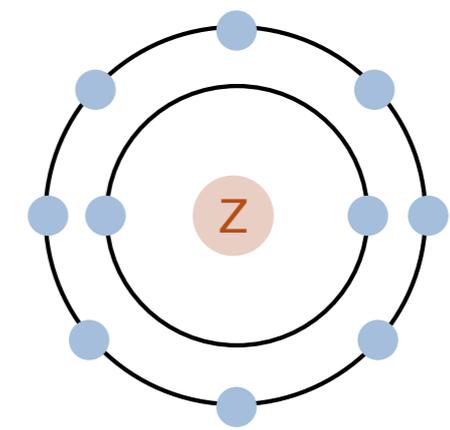
*Used to rationalize the apparent negative charge of electrons with the neutrality of free atoms*



**Rutherford Model - 1911**

An area of high positive charge density surrounded by electrons

*The Geiger-Marsden Experiment (1909) suggested an area of especially high density within the atom, Rutherford then developed this Nuclear Model*

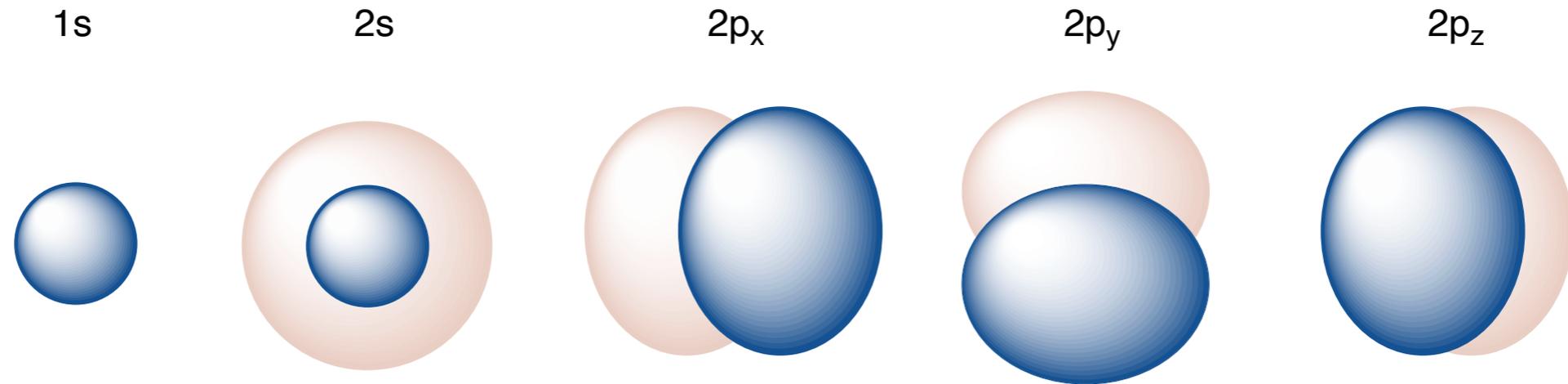


**Bohr Model - 1913**

Electrons orbiting a nucleus in discrete, well-defined orbits

*While more accurate than previous models, physicist couldn't rationalize why electron orbits wouldn't decay*

# History of Atomic Structure

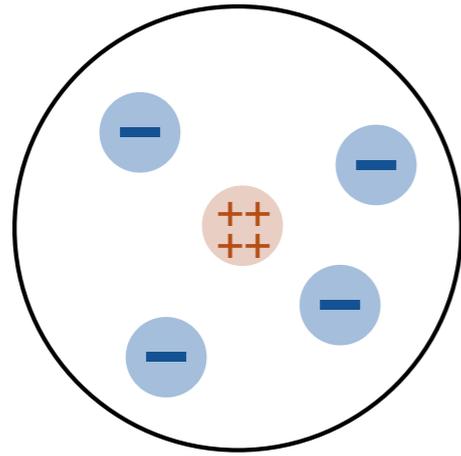


## The Quantum Mechanical Model

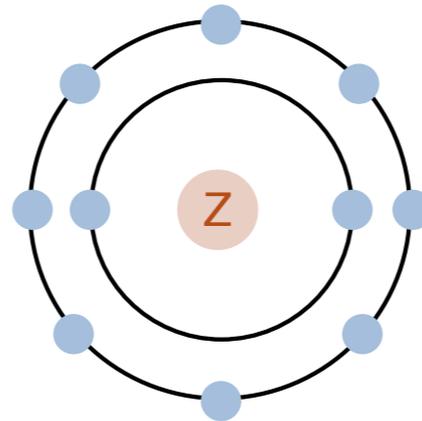
Discrete shells of electrons, with behavior defined by quantum numbers

*In chemistry, we traditionally learn about the history of the model of the atom, but rarely cover the model of the nucleus!*

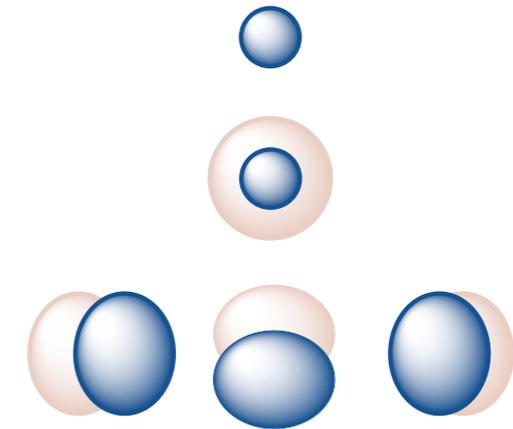
# The Nuclear Model



Rutherford

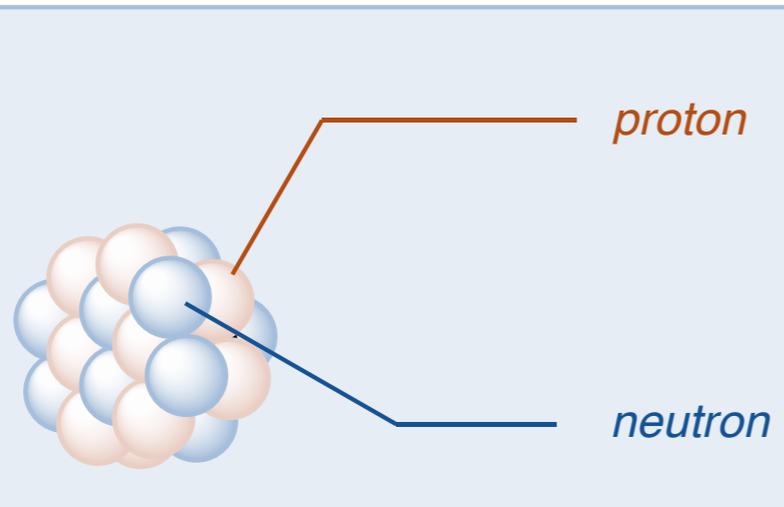


Bohr



Quantum Mechanical

changes in how we think about electron configuration, and thus chemical reactivity



The diagram shows a cluster of spheres representing a nucleus. One sphere is highlighted in orange and labeled 'proton' with a brown line. Another sphere is highlighted in blue and labeled 'neutron' with a blue line. The entire cluster is labeled 'The Nucleus' at the bottom left.

*The Nucleus*

What dictates nuclear structure?  
How does nuclear structure vary between atoms?  
Between isotopes? Between Isomers?  
What makes a stable nucleus?

## Talk Outline

*Brief Review of the Atomic Model*

**Brief Overview: The Standard Model of Particle Physics**

*The Strong and Residual Strong Interactions*

**The Nuclear Shell Model**

*by analogy to the atomic shell model*

**Nuclear Isomers**

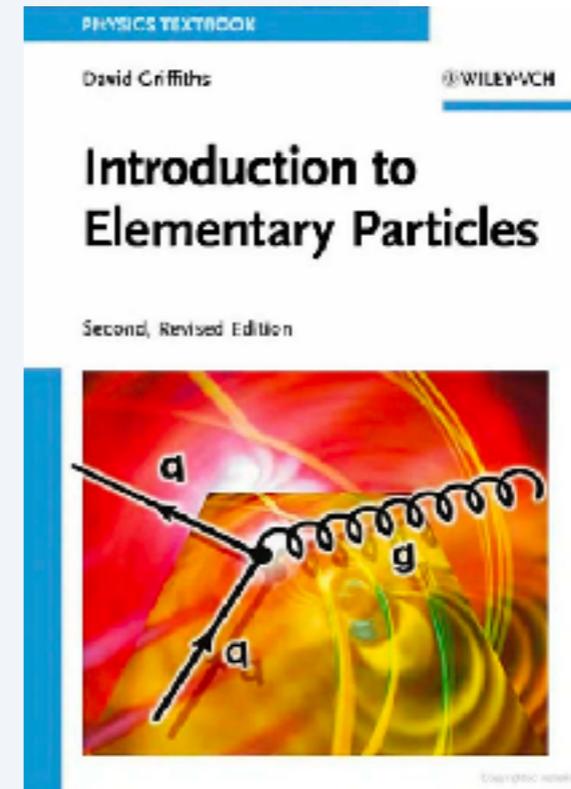
*case studies:*

$^{80m}\text{Br}$

$^{180m}\text{Ta}$

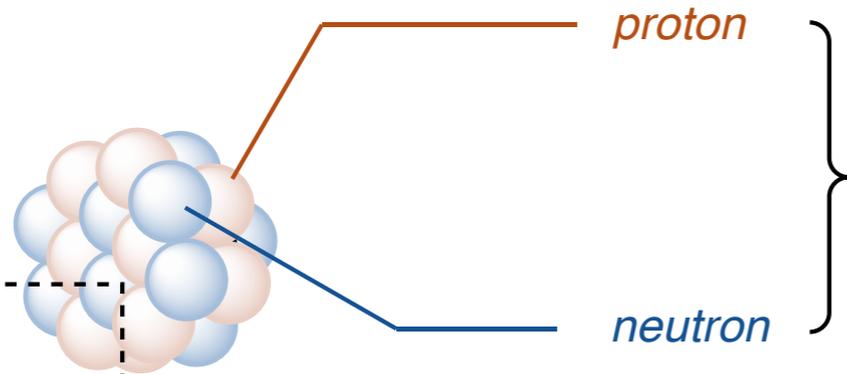
$^{99m}\text{Tc}$

$^{229m}\text{Th}$



# The Standard Model - An Overview

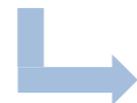
● — *electron* — elementary particle (lepton)



} *not elementary particles!* (hadron - baryon)

**Lepton:** An elementary particle of half integer spin that does not undergo strong interactions

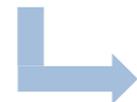
**Hadron:** A subatomic particle comprised of two or more quarks



**Baryon:** A hadron made up of an odd number of quarks

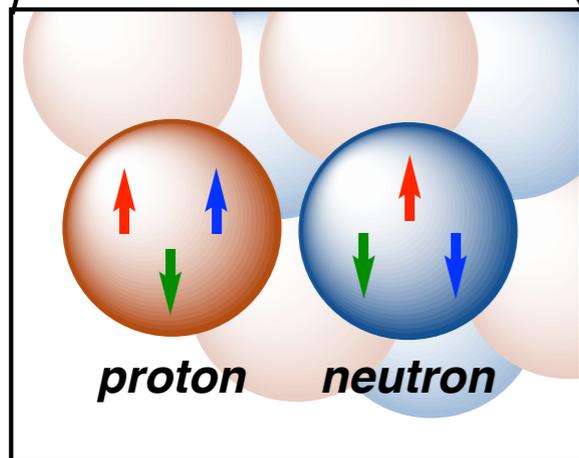
**Meson:** A hadron made up of an even number of quarks

**Quark:** An elementary particle that experiences all four fundamental interactions



**Up quark:** An elementary particle with charge  $+\frac{2}{3}$  and spin  $\frac{1}{2}$

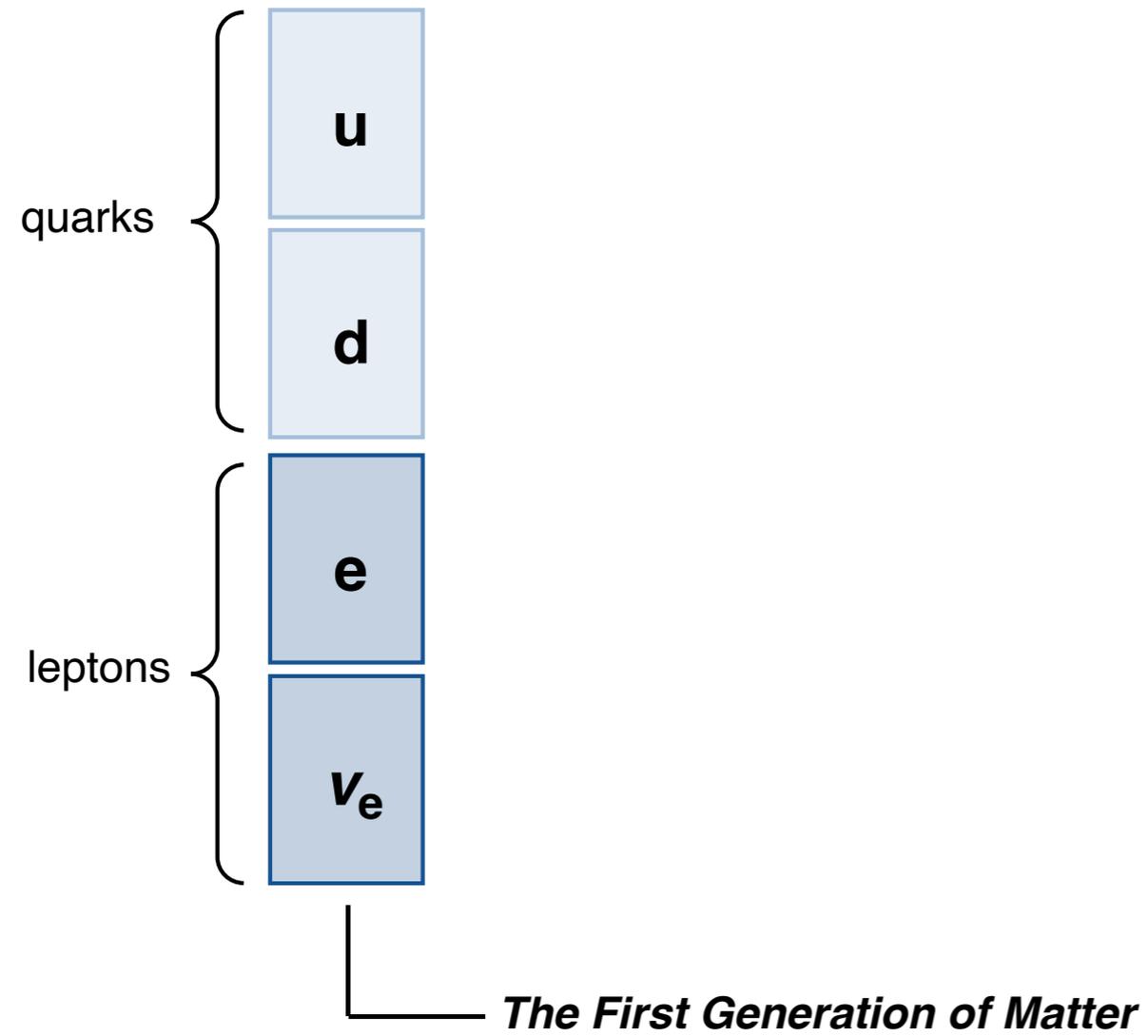
**Down quark:** An elementary particle with charge  $-\frac{1}{3}$  and spin  $\frac{1}{2}$



*Quarks are the origin of proton and neutron charge and spin*

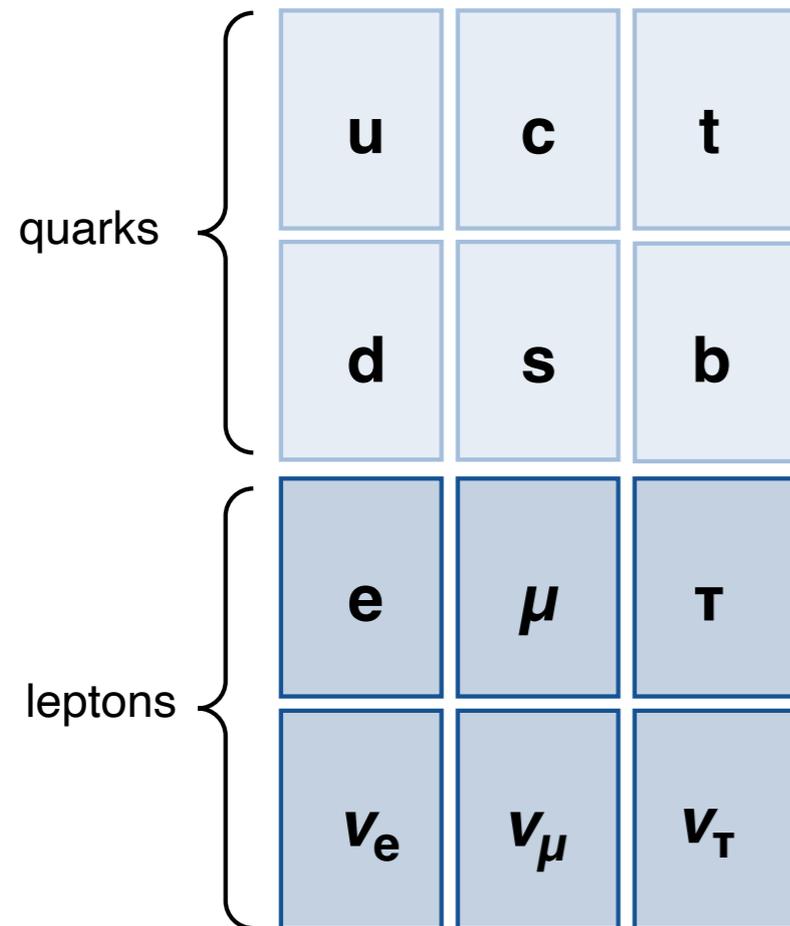
# *The Standard Model - An Overview*

## *Elementary Particles*



# The Standard Model - An Overview

## Elementary Particles



**The Second and Third Generations of Matter**

Heavier, substantially less stable “cousins” of first generation matter. Only detected in cosmic rays or LHC collisions

*Confusing to physicist as to why these exist*

# The Standard Model - An Overview

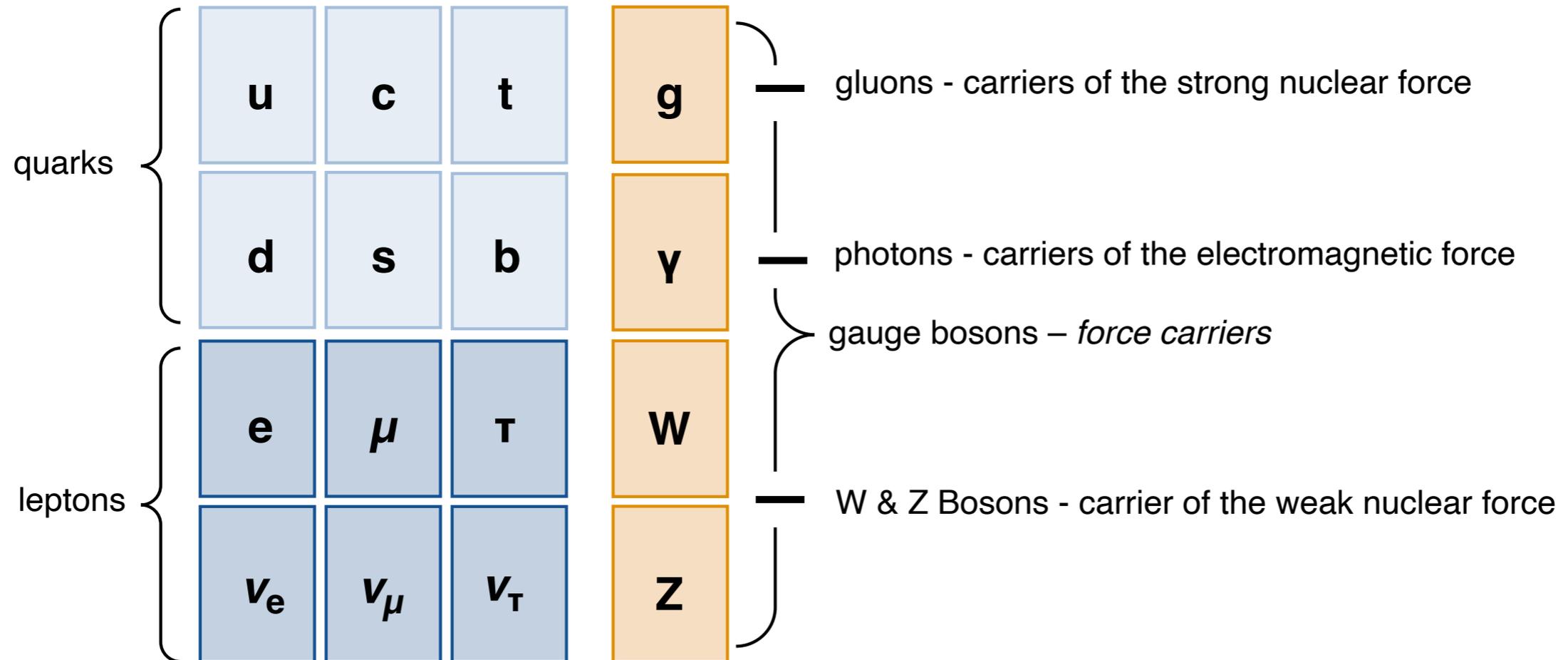
## Elementary Particles

quarks	<b>u</b>	<b>c</b>	<b>t</b>
	<b>d</b>	<b>s</b>	<b>b</b>
leptons	<b>e</b>	<b><math>\mu</math></b>	<b><math>\tau</math></b>
	<b><math>\nu_e</math></b>	<b><math>\nu_\mu</math></b>	<b><math>\nu_\tau</math></b>

***These “matter particles” or fermions are what the universe is made of, but do not explain how or why matter interacts the way it does***

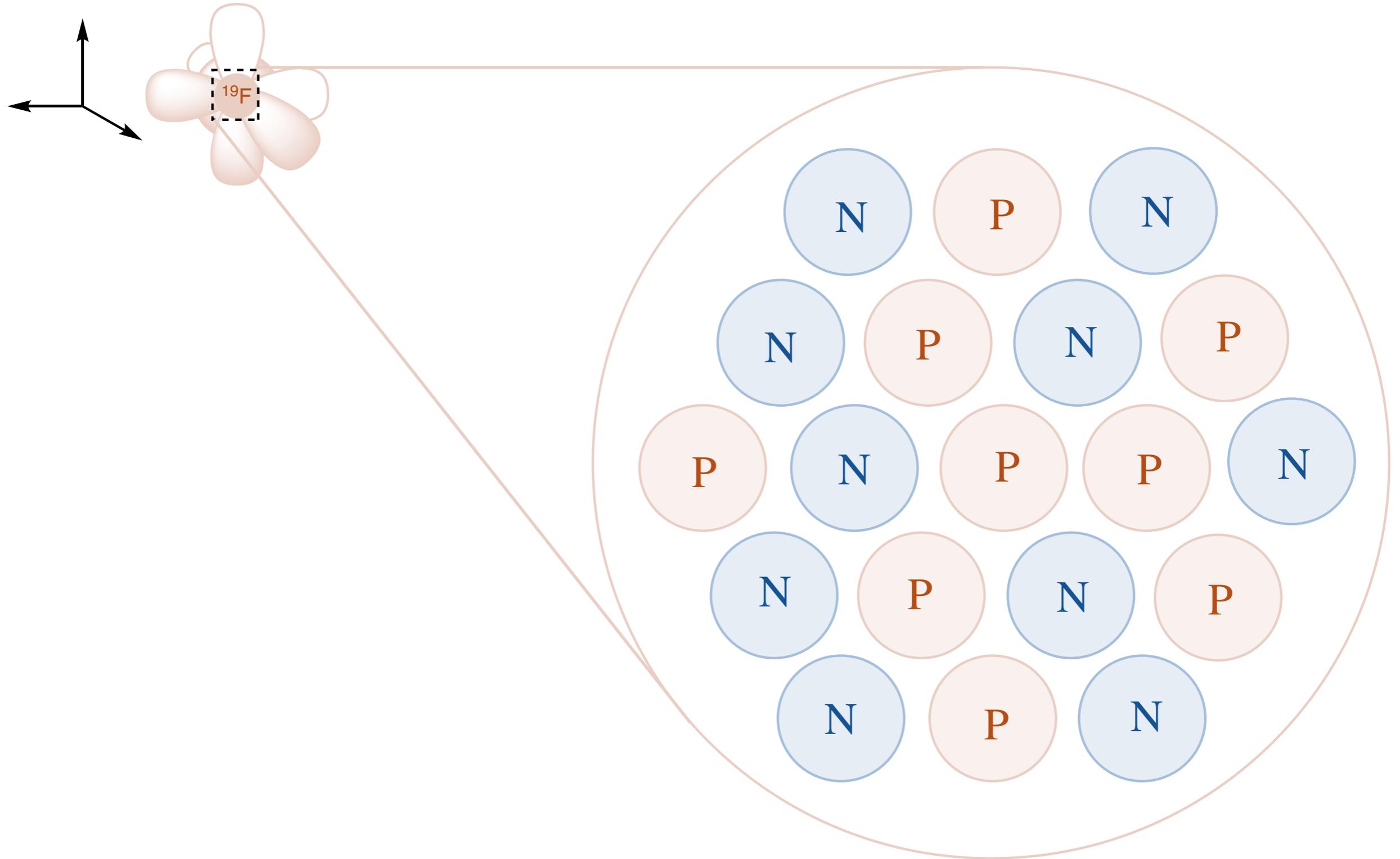
# The Standard Model - An Overview

## Elementary Particles

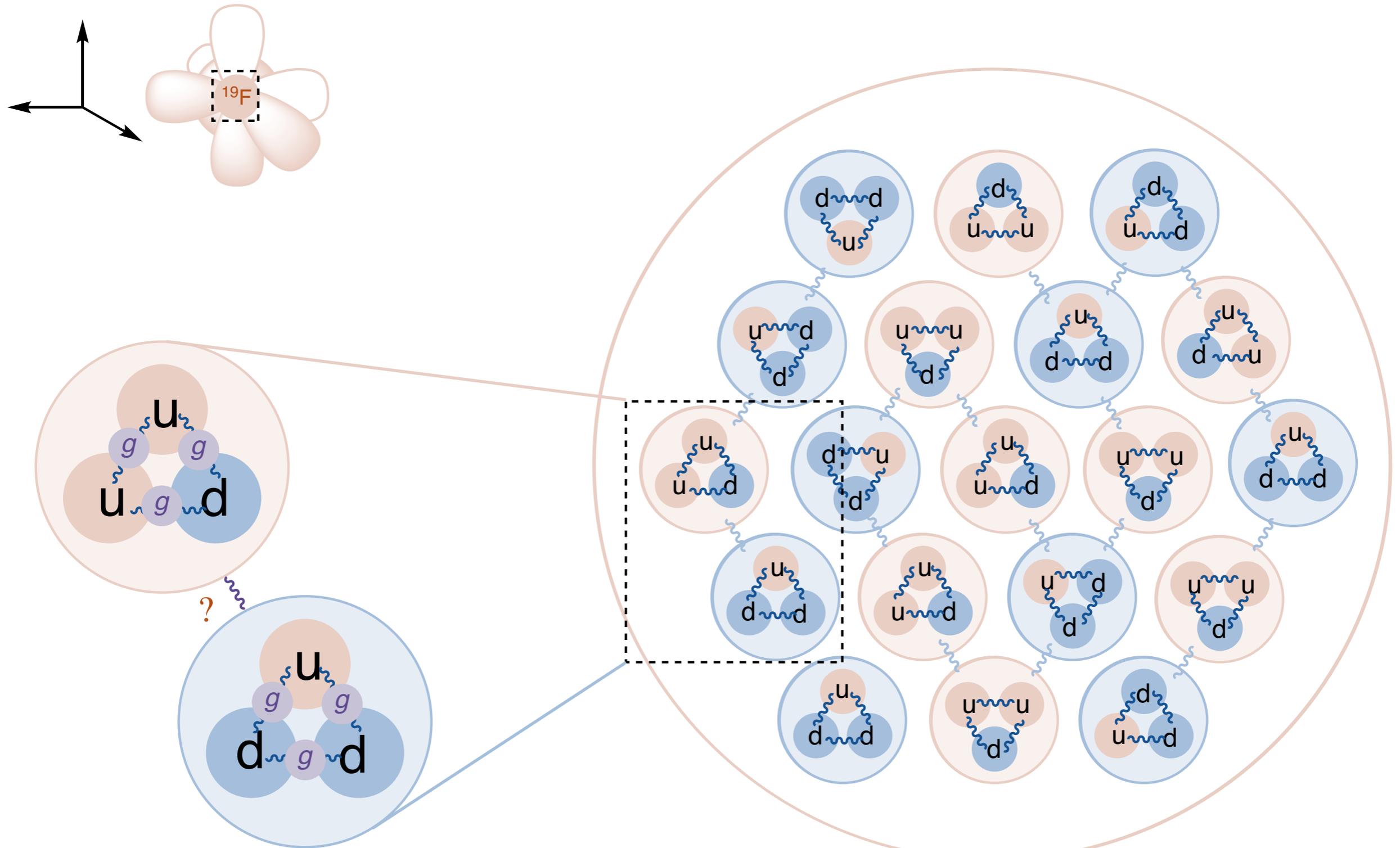


**Particle physics still cannot accurately account for gravitational effects**

# Implications of the Standard Model

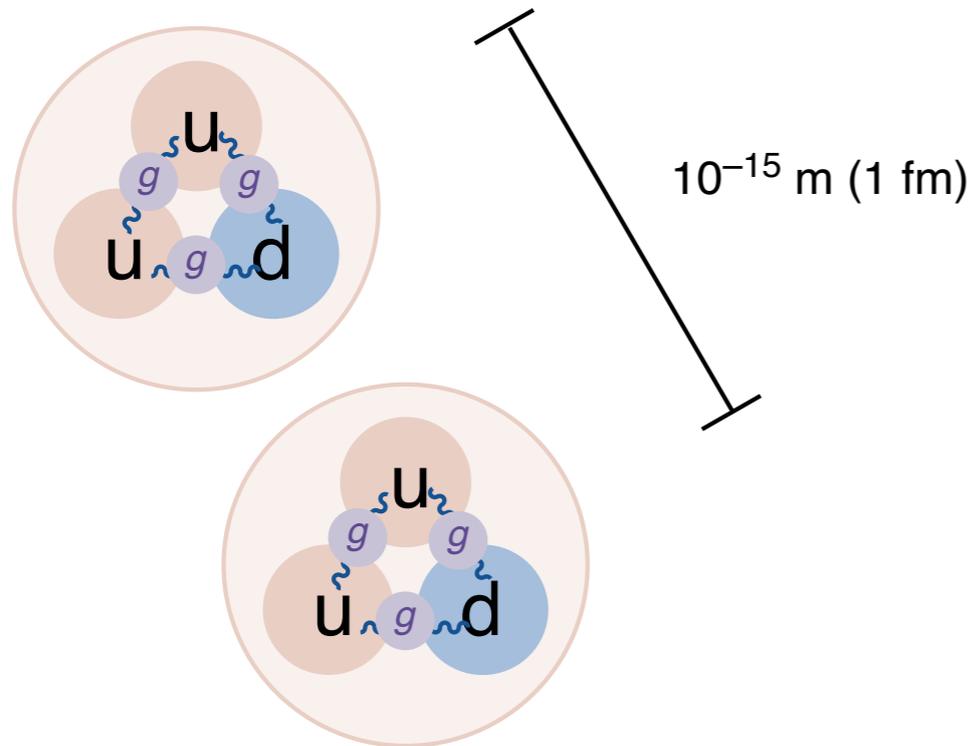


# Implications of the Standard Model



gluon exchange between quarks  
"the strong interaction"

## The Strong Force and the Residual Strong Force

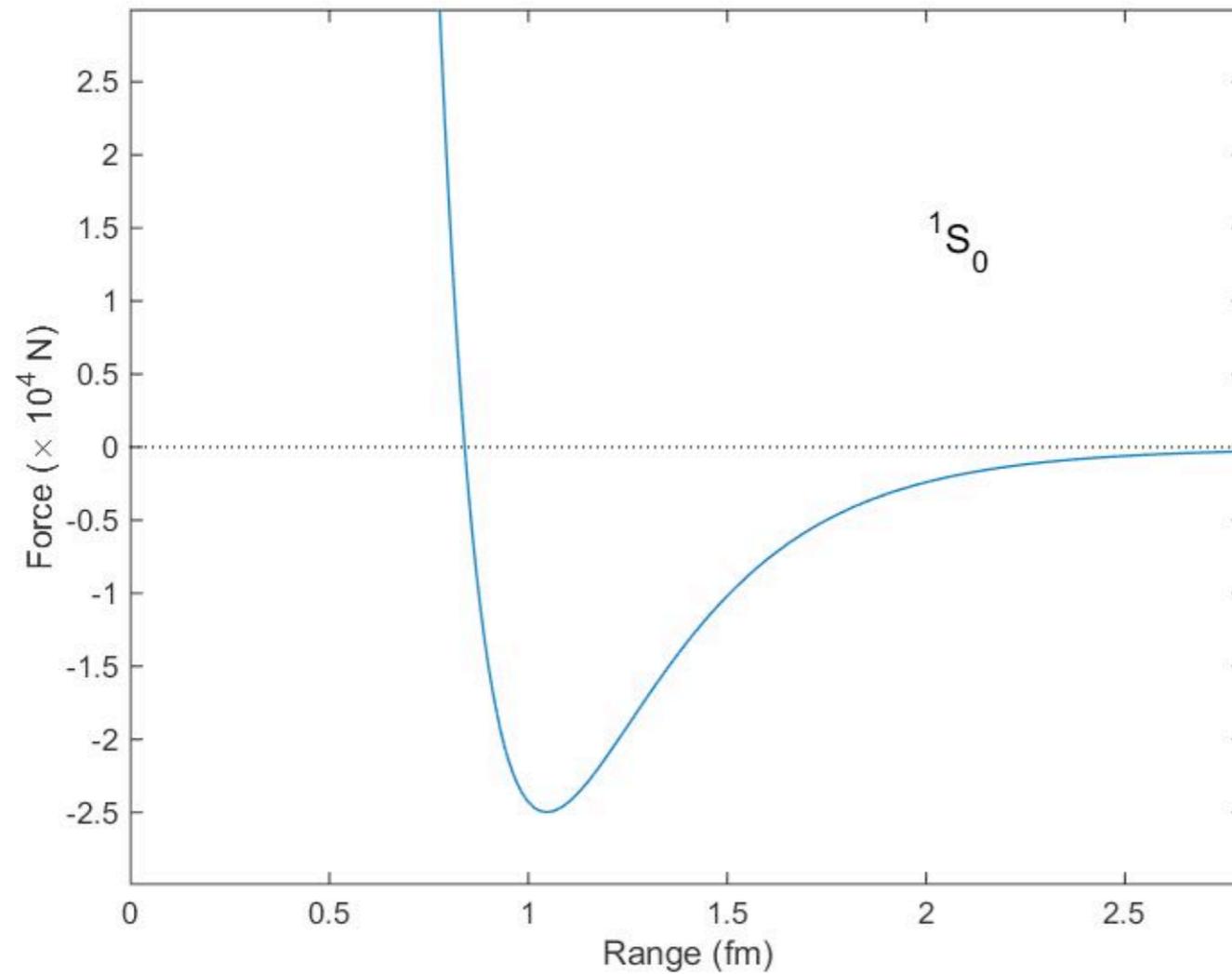


$$F(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r^2}$$

**230 Newtons**

**How does nature overcome this insane barrier? *The Residual Nuclear Force***

## The Strong Force and the Residual Strong Force

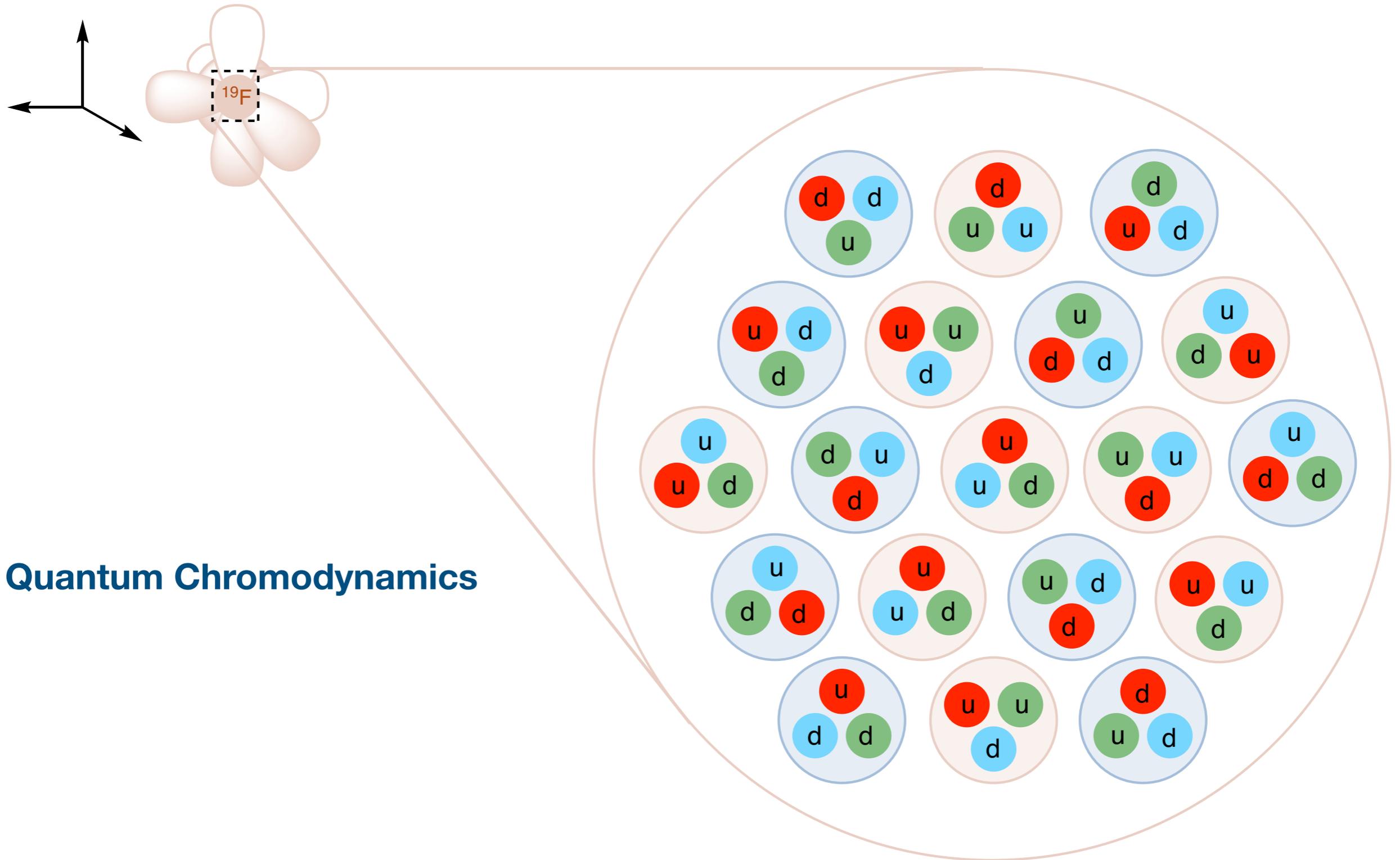


**25000 Newtons**



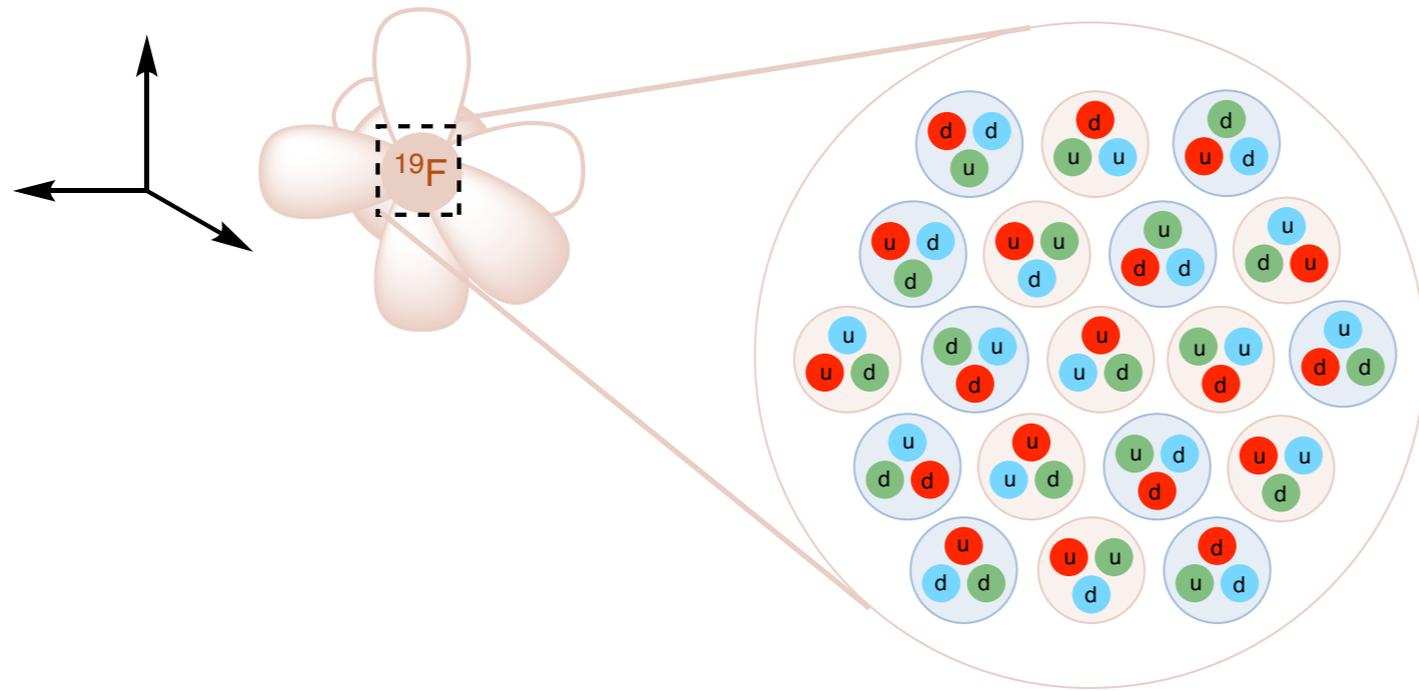
***Can gluons exchange between quarks confined within different Baryons?***

# A (Very) Brief Intro to QCD



**Quantum Chromodynamics**

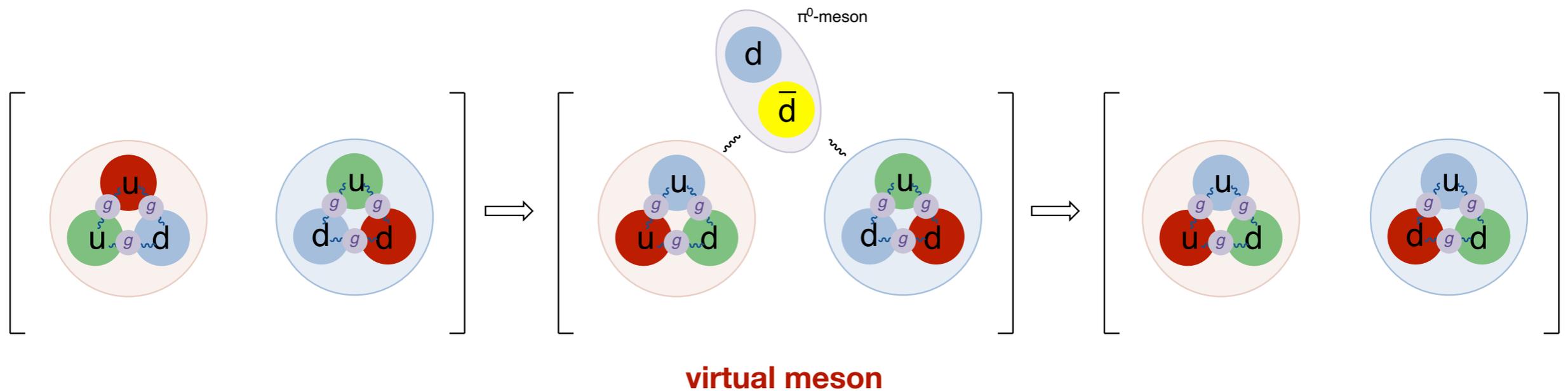
# A (Very) Brief Intro to QCD



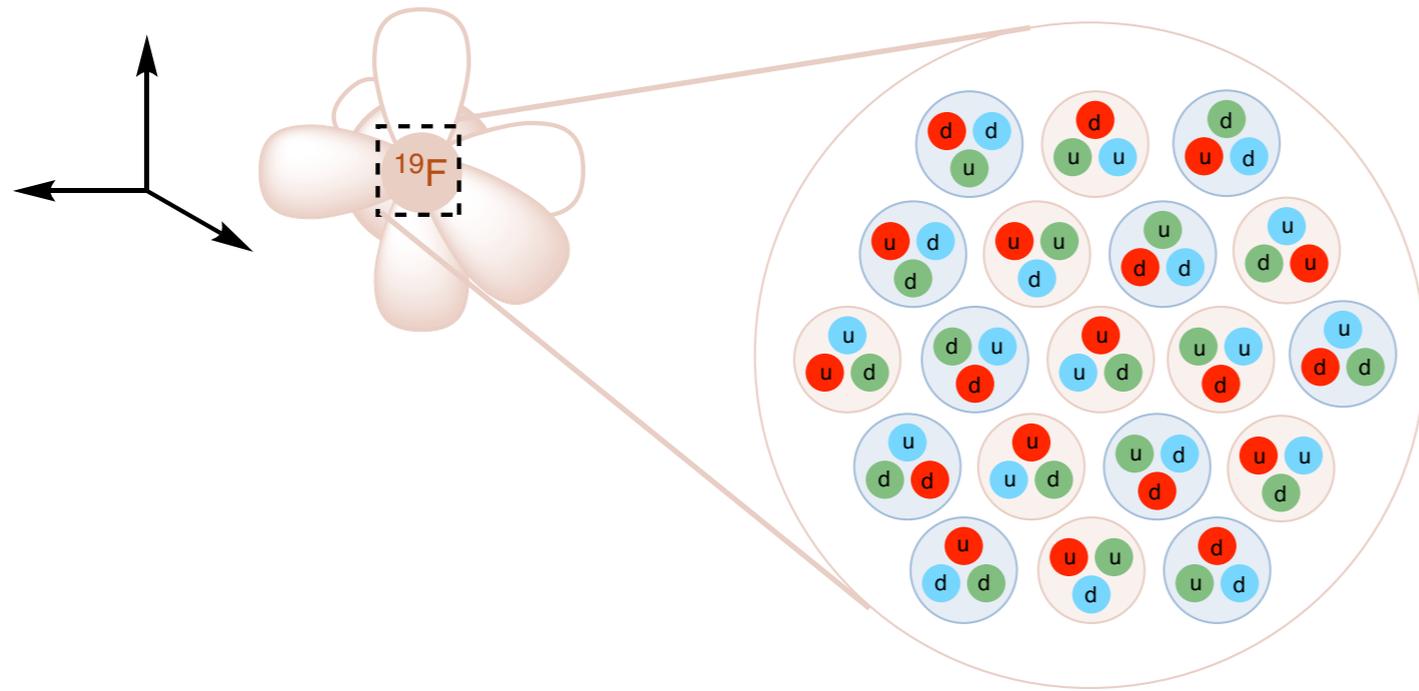
Three “colors” of strong force “charges;” each attracted to the other two by exchange of gluons

The force required to separate two quarks of a different color grows proportionally to the distance between them

Eventually, enough energy is put in to create a new quark pair, separate from the hadron



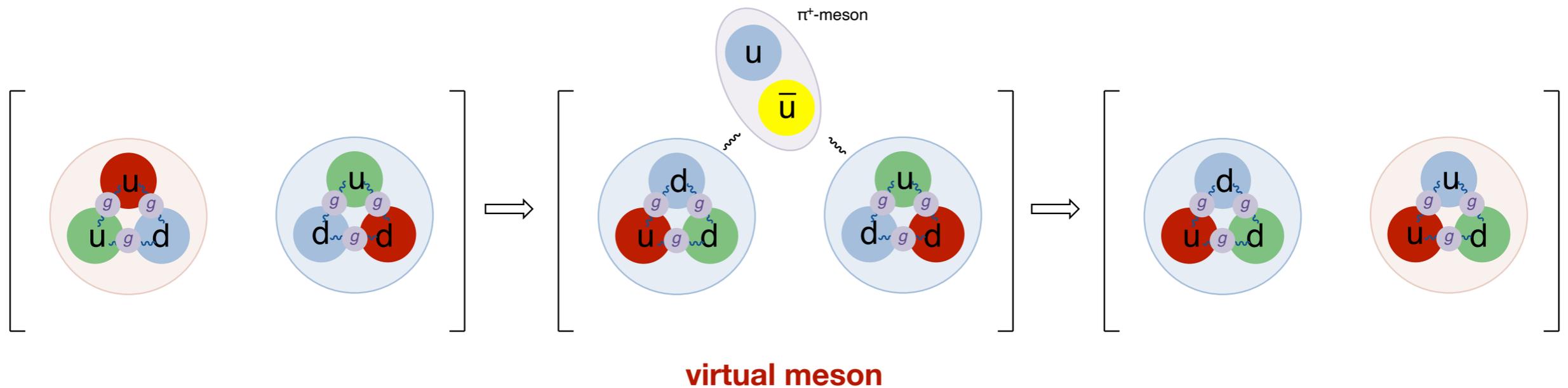
# A (Very) Brief Intro to QCD



Three “colors” of strong force “charges;” each attracted to the other two by exchange of gluons

The force required to separate two quarks of a different color grows proportionally to the distance between them

Eventually, enough energy is put in to create a new quark pair, separate from the hadron



# The Nuclear Shell Model by Analogy to the Atomic Shell Model

- **A brief review of the atomic shell model:**

*Four quantum numbers define an electron in an atom*

$n$  – principle quantum number, the energy level of the electron. Integer value from 1 to infinity

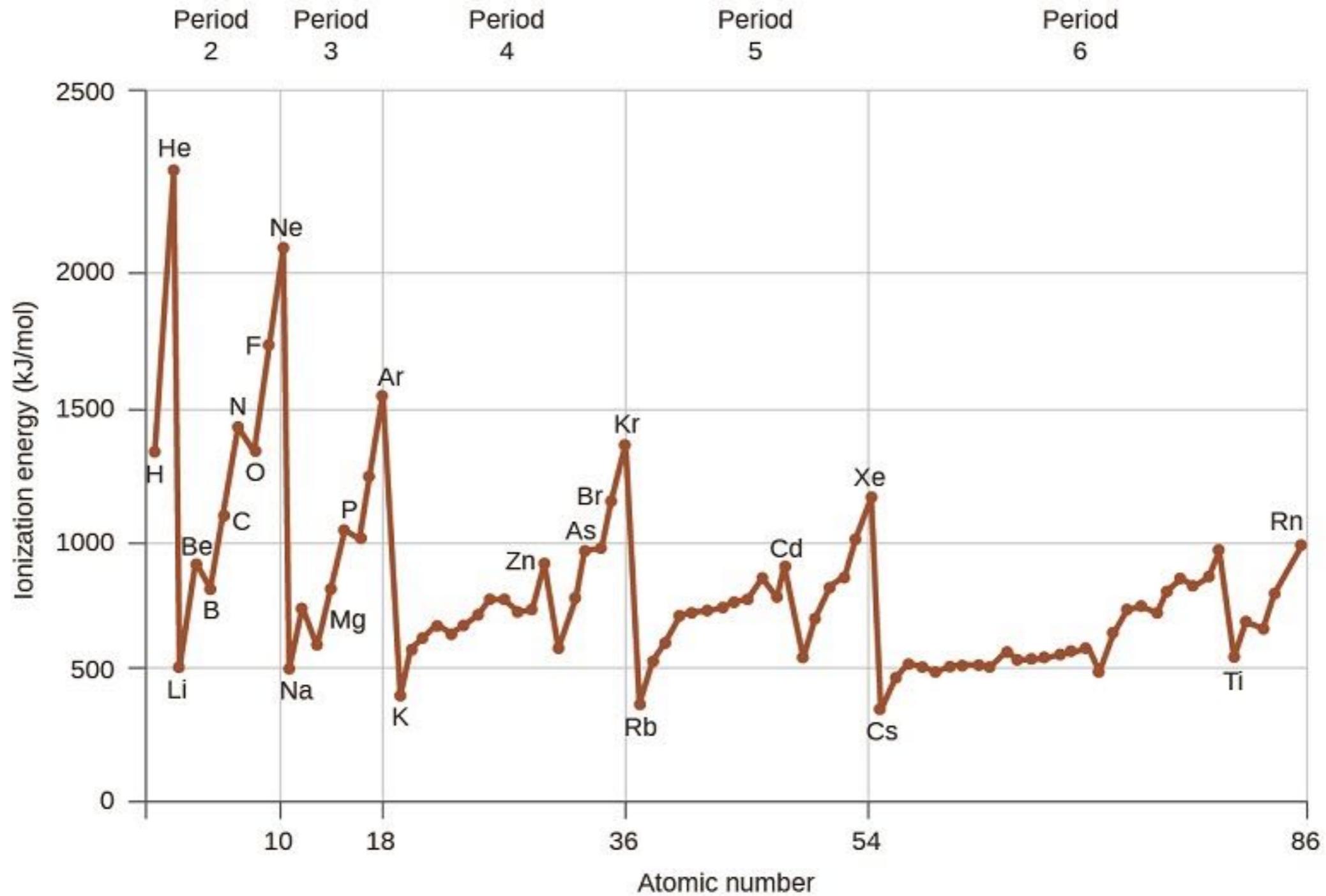
$l$  – angular momentum quantum number, ranges from 0 to  $n-1$ . 0 = s, 1 = p, 2 = d, 3 = f, etc.

$m_l$  – magnetic quantum number, ranges from  $-l$  to  $l$ .

$m_s$  – spin quantum number, ranges from  $-s$  to  $s$  ( $\pm 1/2$ )

<b>for <math>n = 1</math>:</b> $l = 0$ $m_l = 0$ $m_s = 1/2$ or $-1/2$	<b>for <math>n = 2</math>:</b> $l = 0$ or $+1$ $m_l = -1, 0,$ or $+1$ (for $m \neq 0$ ) $m_s = 1/2$ or $-1/2$	<b>for <math>n = 3</math>:</b> $l = 0, +1, +2$ $m_l = -2, -1, 0, +1, +2$ (for $m=2$ ) $m_s = 1/2$ or $-1/2$
<b>2</b>	<b>2 + 6</b>	<b>2 + 6 + 10</b>
<b>2 = He</b>	<b>10 = Ne</b> <b>18 = Ar</b>	<b>36 = Kr</b>

# The Nuclear Shell Model by Analogy to the Atomic Shell Model



# The Nuclear Shell Model

- **Application to the Nuclear Shell Model**

*Four quantum numbers define a Nucleon, with Neutrons and Protons treated independently*

$n$  – principle quantum number, the energy level of the electron. Integer value from 1 to infinity

$l$  – angular momentum quantum number, **not restricted by  $n$**

$m_l$  – magnetic quantum number, ranges from  $-l$  to  $l$ .

$m_s$  – spin quantum number, ranges from  $-s$  to  $s$  ( $\pm 1/2$ )

*This treatment affords filled shell numbers of **2, 8, 20, 28, 50, 82, 126***

*Magic nuclei: Nuclei with an atomic number or neutron number that is “magic” (a filled shell) ( $^{58}\text{Ni}$ )*

*Doubly magic nuclei: Nuclei with both an atomic number and neutron number that is “magic” ( $^{48}\text{Ni}$ )*

# The Nuclear Shell Model

$^{40}\text{Ca}$  - heaviest stable nuclide where  $N = Z$

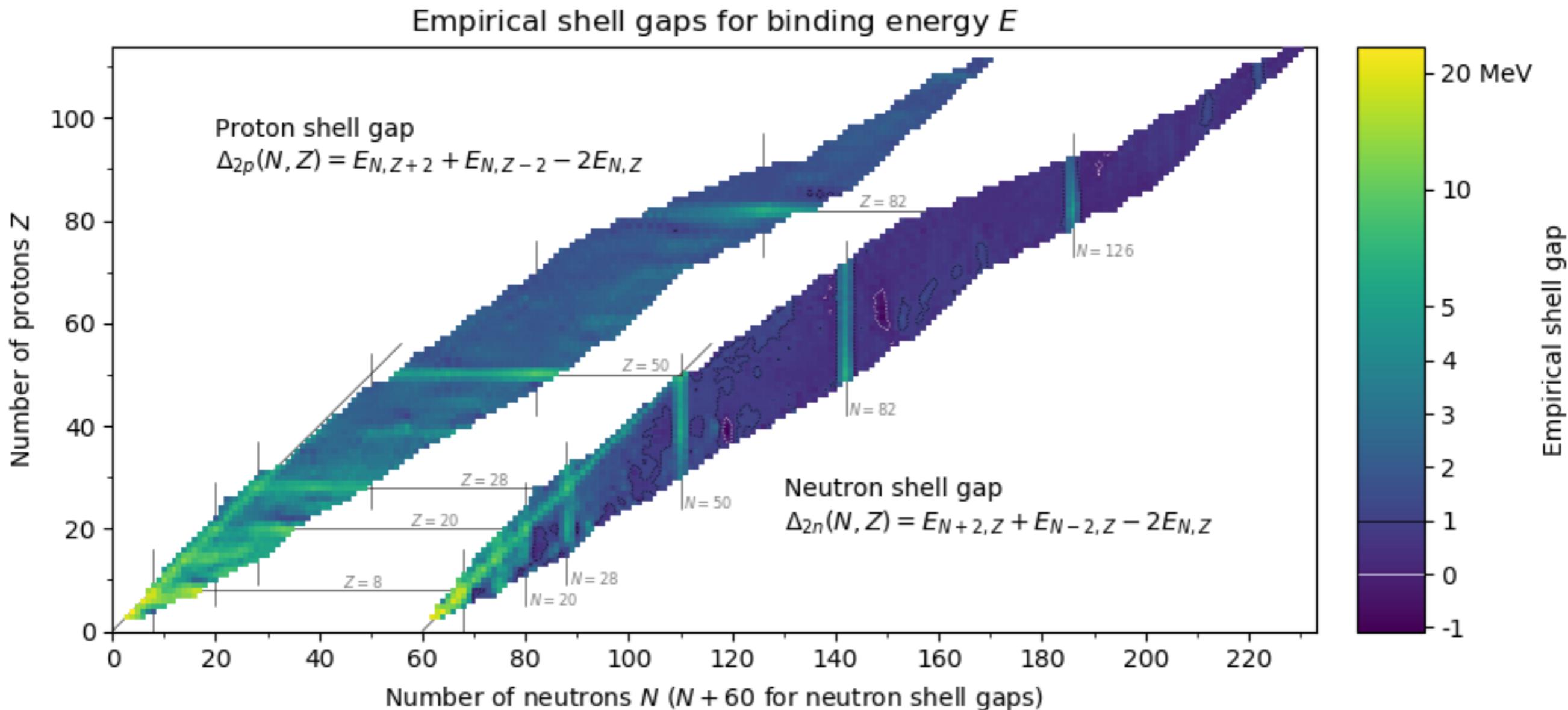
$^{48}\text{Ni}$  - the most proton rich nuclide beyond  $^3\text{He}$  ( $28 + 20$ )

$^{78}\text{Ni}$  - extremely high neutron ratio, thought to be important in stellar nucleosynthesis

$^{10}\text{He}$  is doubly-magic ( $10^3$  longer lived than  $^5\text{He}$ )

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		**	89 <b>Ac</b> Actinium Actinide	90 <b>Th</b> Thorium Actinide	91 <b>Pa</b> Protactinium Actinide	92 <b>U</b> Uranium Actinide	93 <b>Np</b> Neptunium Actinide	94 <b>Pu</b> Plutonium Actinide	95 <b>Am</b> Americium Actinide	96 <b>Cm</b> Curium Actinide	97 <b>Bk</b> Berkelium Actinide	98 <b>Cf</b> Californium Actinide	99 <b>Es</b> Einsteinium Actinide	100 <b>Fm</b> Fermium Actinide	101 <b>Md</b> Mendelevium Actinide	102 <b>No</b> Nobelium Actinide	103 <b>Lr</b> Lawrencium Actinide						

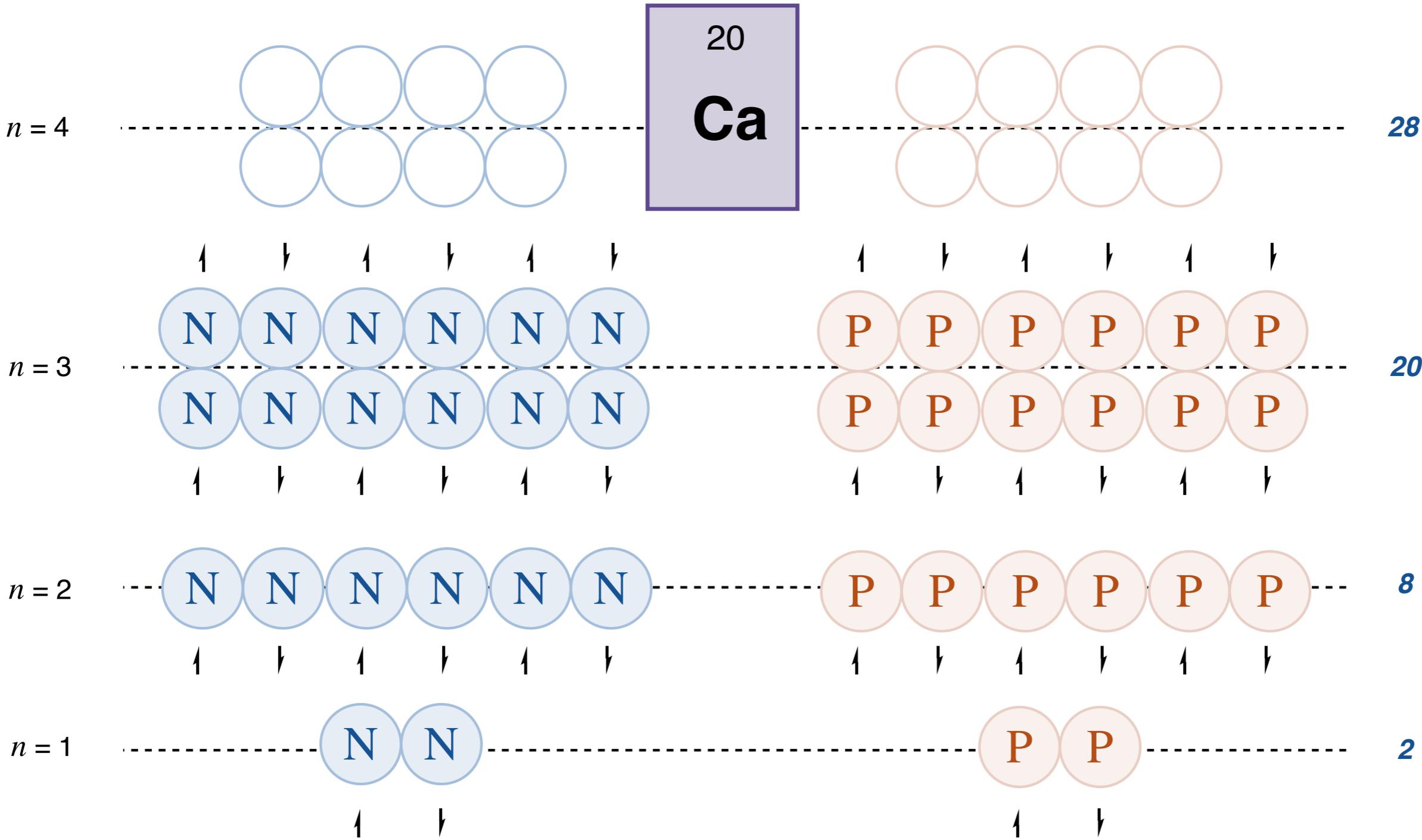
# The Nuclear Shell Model



Magic numbers are calculated only for *spherical nuclei*

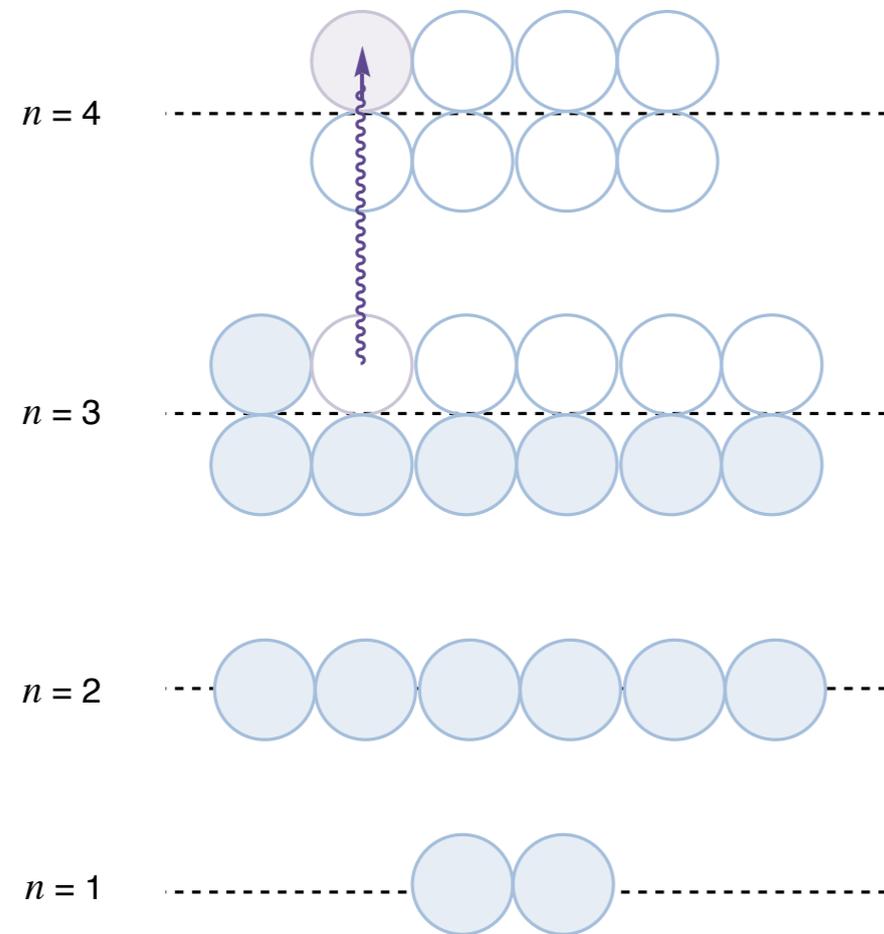
Magic numbers (or semi-magic numbers) can be empirically derived from these tables

# The Nuclear Shell Model

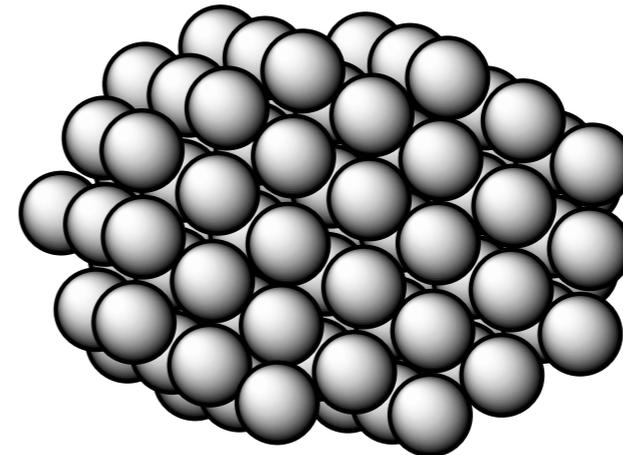


# Nuclear Excited States

## Nuclear Transition (Shell Theory)



## Vibrational and Rotational Excitation in Deformed Nuclei (Collective Theory)



# The Nuclear Shell Model

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87 <b>Fr</b> Francium Alkali Metal	88 <b>Ra</b> Radium Alkaline Earth Metal	**	104 <b>Rf</b> Rutherfordium Transition Metal	105 <b>Db</b> Dubnium Transition Metal	106 <b>Sg</b> Seaborgium Transition Metal	107 <b>Bh</b> Bohrium Transition Metal	108 <b>Hs</b> Hassium Transition Metal	109 <b>Mt</b> Meitnerium Transition Metal	110 <b>Ds</b> Darmstadtium Transition Metal	111 <b>Rg</b> Roentgenium Transition Metal	112 <b>Cn</b> Copernicium Transition Metal	113 <b>Nh</b> Nihonium Post-Transition Metal	114 <b>Fl</b> Flerovium Post-Transition Metal	115 <b>Mc</b> Moscovium Post-Transition Metal	116 <b>Lv</b> Livermorium Post-Transition Metal	117 <b>Ts</b> Tennessine Halogen	118 <b>Og</b> Oganesson Noble Gas						
		*	57 <b>La</b> Lanthanum Lanthanide	58 <b>Ce</b> Cerium Lanthanide	59 <b>Pr</b> Praseodymium Lanthanide	60 <b>Nd</b> Neodymium Lanthanide	61 <b>Pm</b> Promethium Lanthanide	62 <b>Sm</b> Samarium Lanthanide	63 <b>Eu</b> Europium Lanthanide	64 <b>Gd</b> Gadolinium Lanthanide	65 <b>Tb</b> Terbium Lanthanide	66 <b>Dy</b> Dysprosium Lanthanide	67 <b>Ho</b> Holmium Lanthanide	68 <b>Er</b> Erbium Lanthanide	69 <b>Tm</b> Thulium Lanthanide	70 <b>Yb</b> Ytterbium Lanthanide	71 <b>Lu</b> Lutetium Lanthanide						
		**	89 <b>Ac</b> Actinium Actinide	90 <b>Th</b> Thorium Actinide	91 <b>Pa</b> Protactinium Actinide	92 <b>U</b> Uranium Actinide	93 <b>Np</b> Neptunium Actinide	94 <b>Pu</b> Plutonium Actinide	95 <b>Am</b> Americium Actinide	96 <b>Cm</b> Curium Actinide	97 <b>Bk</b> Berkelium Actinide	98 <b>Cf</b> Californium Actinide	99 <b>Es</b> Einsteinium Actinide	100 <b>Fm</b> Fermium Actinide	101 <b>Md</b> Mendelevium Actinide	102 <b>No</b> Nobelium Actinide	103 <b>Lr</b> Lawrencium Actinide						

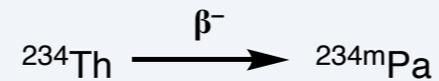
$^{270}\text{Hs}$   
 $Z = 108, N = 162$   
 doubly magic for deformed nuclei

# Nuclear Isomers

Nuclear excited states typically decay within  $10^{-12}$  s

Nuclear excited states that are longer lived than 1 ns ( $10^{-9}$  s) are considered nuclear isomers

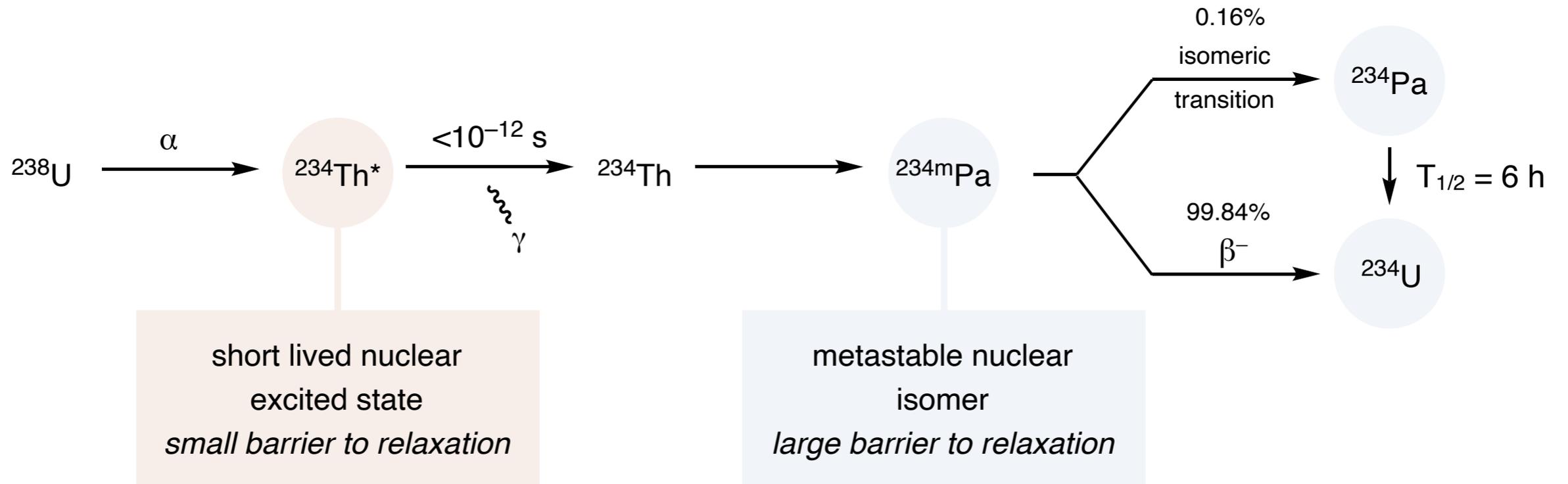
Metastable isomers are traditionally nuclear reaction products that are formed in an excited state (e.g. via the conversion of a neutron to a proton in an unusual spin state)



*protactinium was discovered as its metastable state!* ( $T_{1/2} = 1.17$  minutes)

# Metastable Nuclear Isomers

## Typical decay chain: A case study



### Isomeric transition: Decay of nuclear isomer/excited state to a lower energy state

#### gamma emission

*analogous to electronic excited state  
decay via photon emission*

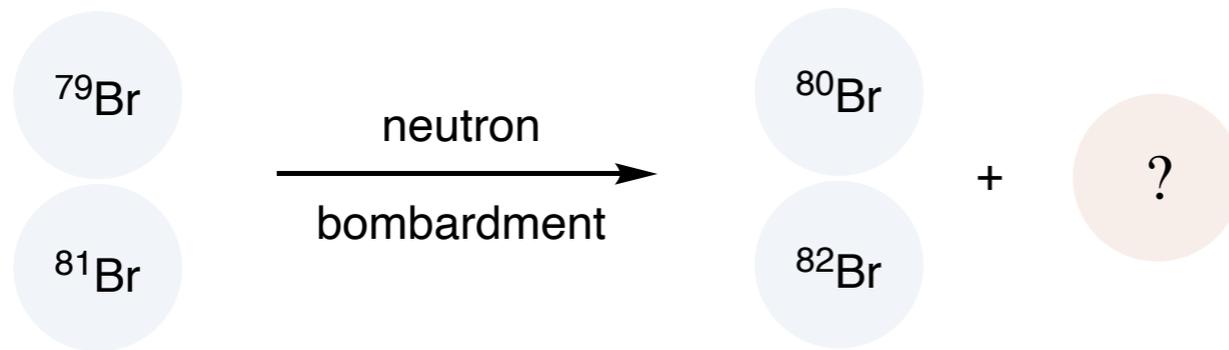
#### internal conversion

*an electron couples to the  
excited nucleus, and relaxation of the  
nucleus ejects the electron  
(note: this is different from  $\beta$  decay)*

## Notable Nuclear Isomers: $^{80m}\text{Br}$

1934: Kurchatov and coworkers publish on the neutron bombardment of a commercial  $\text{Br}_2$  sample.

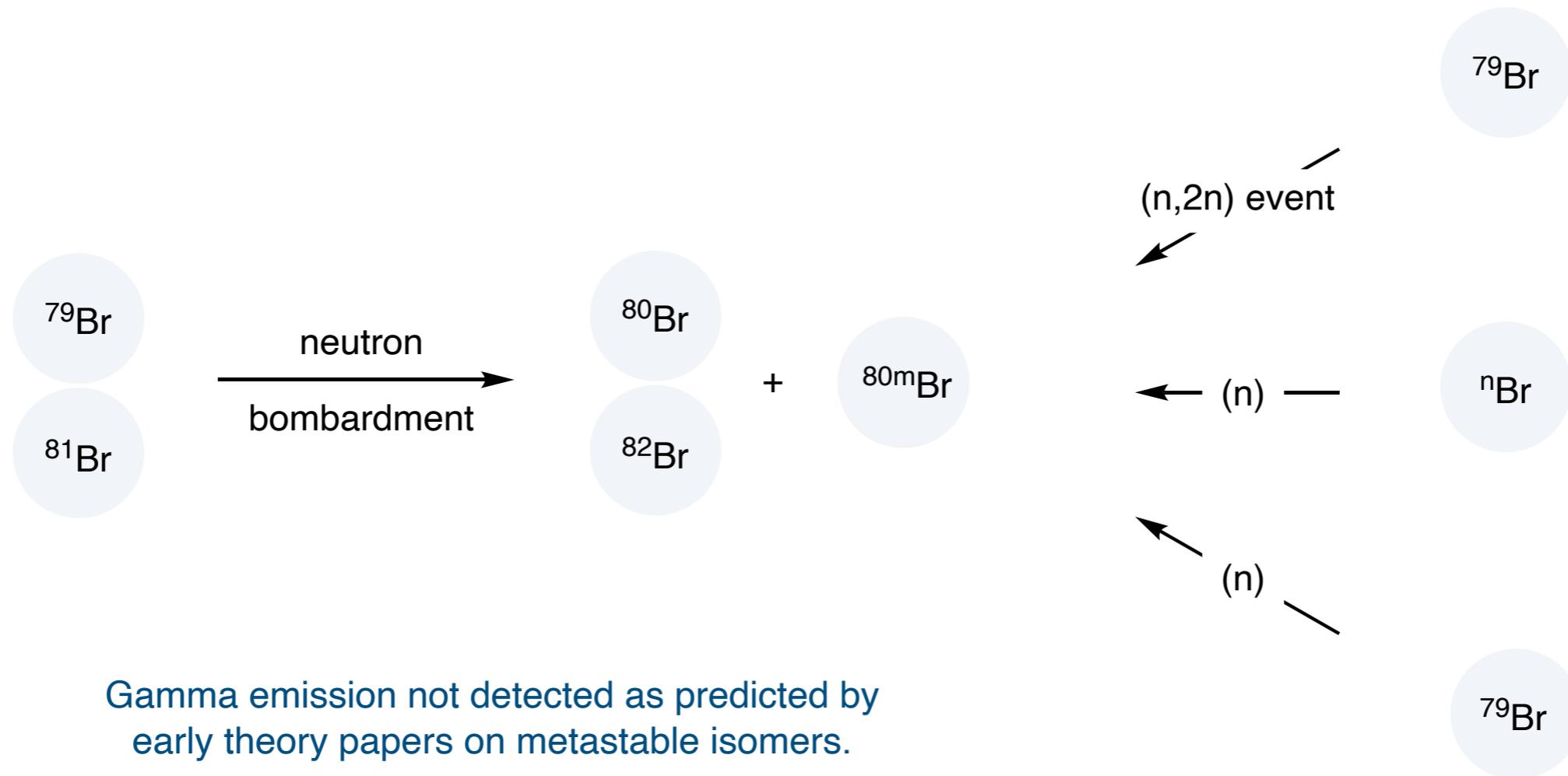
Three distinct beta-emitting isotopes are detected



# Notable Nuclear Isomers: $^{80m}\text{Br}$

1934: Kurchatov and coworkers publish on the neutron bombardment of a commercial  $\text{Br}_2$  sample.

Three distinct beta-emitting isotopes are detected



Gamma emission not detected as predicted by early theory papers on metastable isomers.

Internal conversion mistaken for  $\beta$  decay

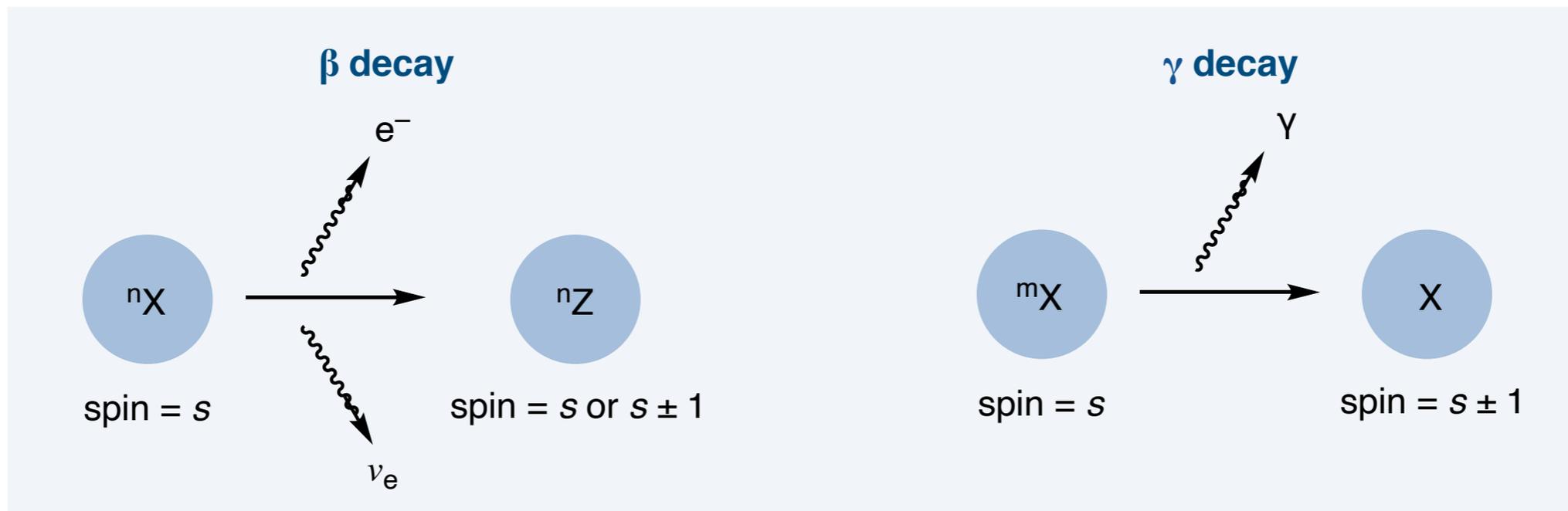
## Notable Nuclear Isomers: $^{180m1}\text{Ta}$

$^{180}\text{Ta}$  is a spin = 1 nucleus with an odd number of both protons and neutrons (odd/odd nucleus)

$T_{1/2} = 8.1$  h: electron capture to  $^{180}\text{Hf}$  or  $\beta^-$  to  $^{180}\text{W}$

$^{180m1}\text{Ta}$ : The rarest primordial nuclide in the universe - observationally stable

$T_{1/2} > 10^{16}$  years



Each additional (forbidden) unit of angular momentum slows the relaxation process by  $10^5$

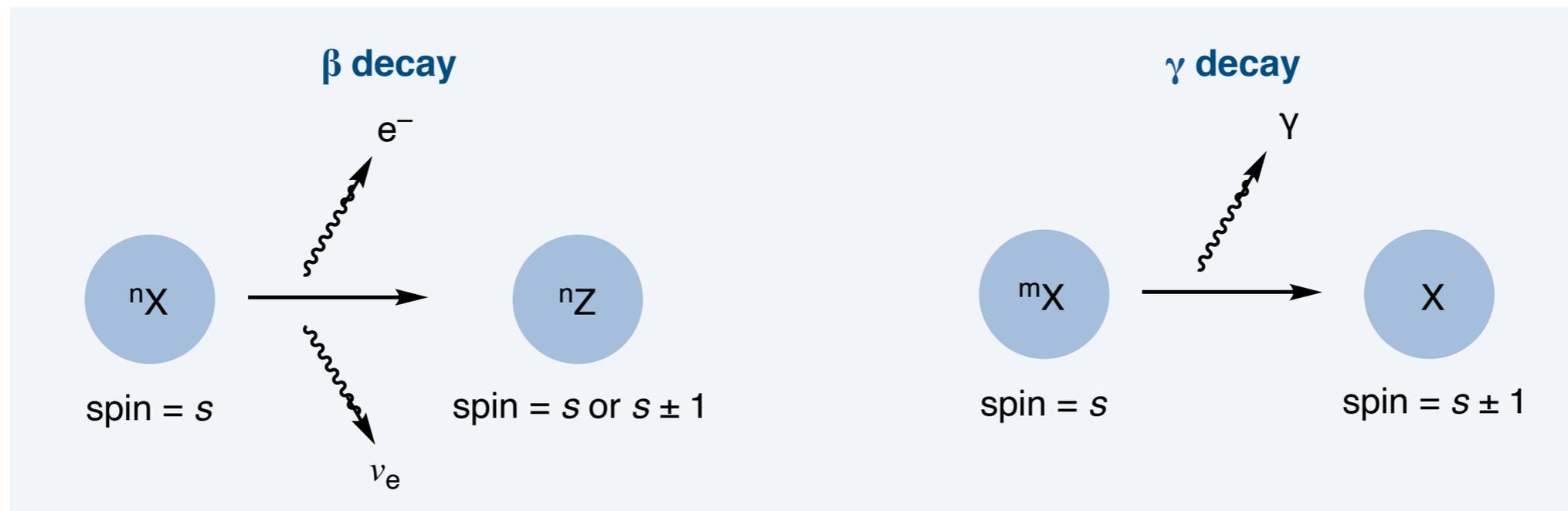
## Notable Nuclear Isomers: $^{180m1}\text{Ta}$

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$^{180m1}\text{Ta}$ : The rarest primordial nuclide in the universe - observationally stable

$T_{1/2} > 10^{16}$  years

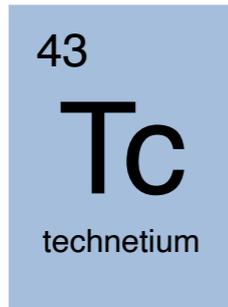


What imparts this exceptional stability against all decay pathways of  $^{180m1}\text{Ta}$ ?

**Nuclear spin = 9! Any decay pathway is “exceptionally forbidden”**

**Rate decrease of  $10^{57}$**

## Notable Nuclear Isomers: $^{99m}\text{Tc}$

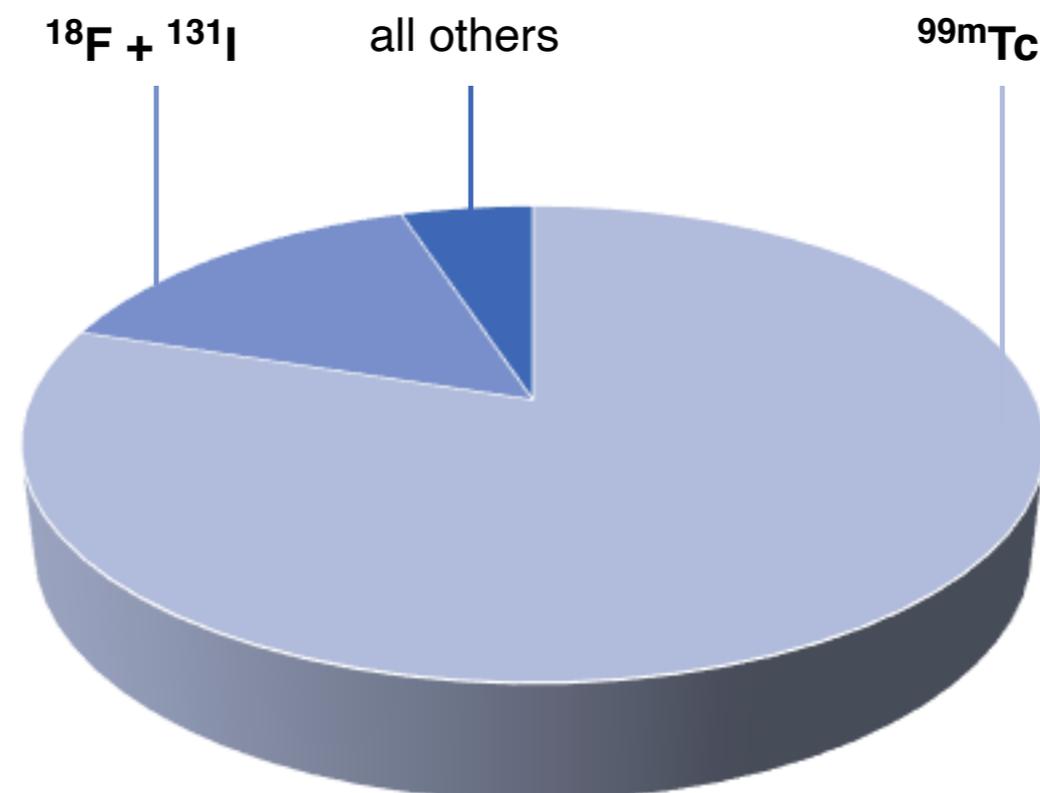


*exceedingly rare as a naturally occurring element due to short half lives of all naturally occurring isotopes (<4.2 My)*

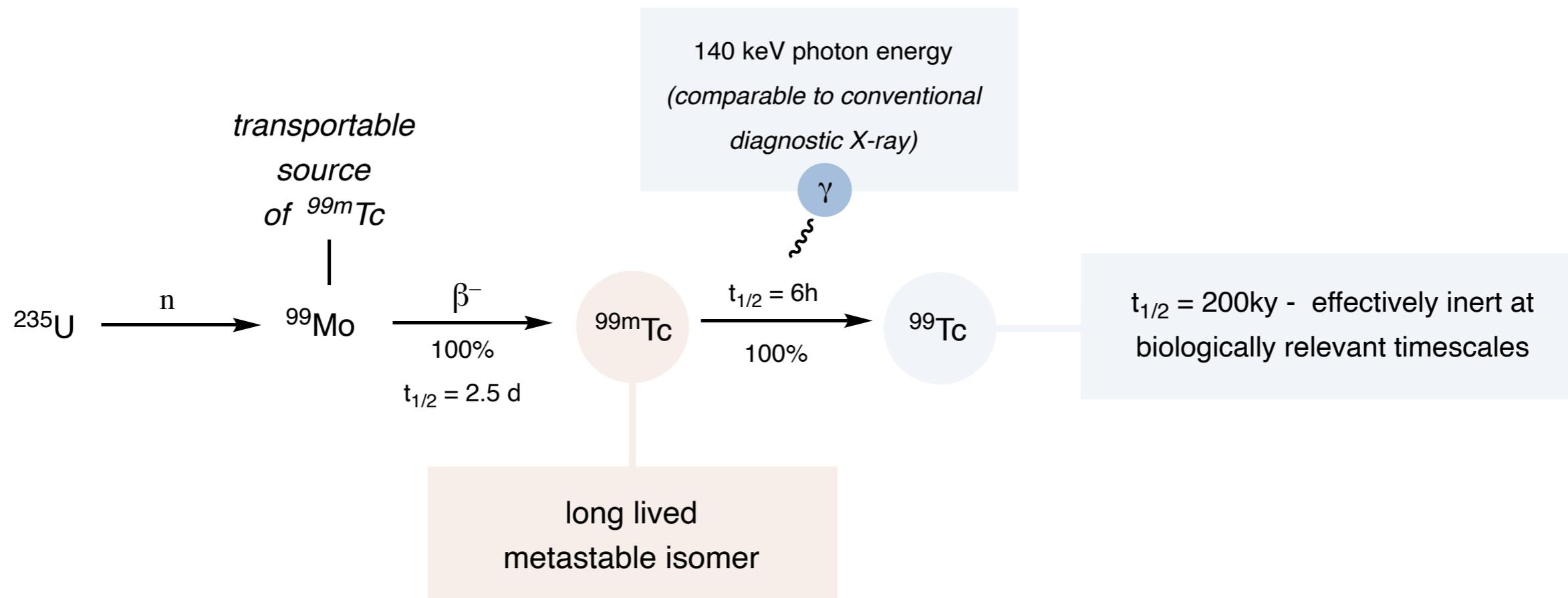
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*all technetium used for radiochemical applications is produced synthetically*

**The metastable isomer  $^{99m}\text{Tc}$  has extensive applications as a medical radioisotope**

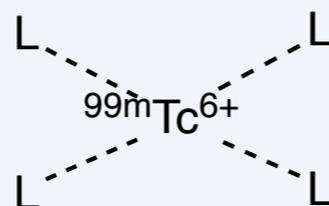
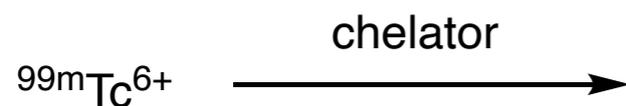


## Notable Nuclear Isomers: $^{99m}\text{Tc}$



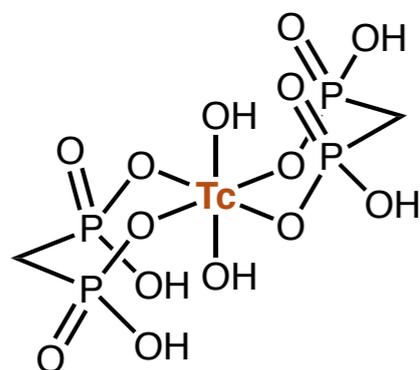
**clean gamma emission only - easily detectable by gamma cameras**  
**no alpha or beta particles *in vivo***

## Notable Nuclear Isomers: $^{99m}\text{Tc}$



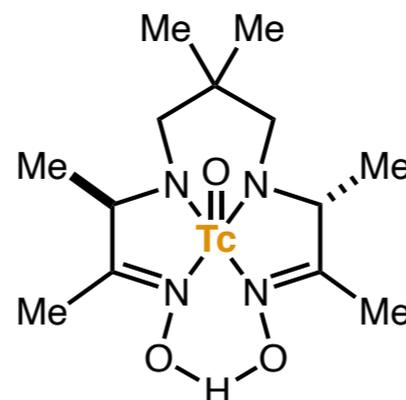
*chelator/ligand sphere is adjusted for specific applications and site specificity*

*purified to >99% RCP with commercial kits*



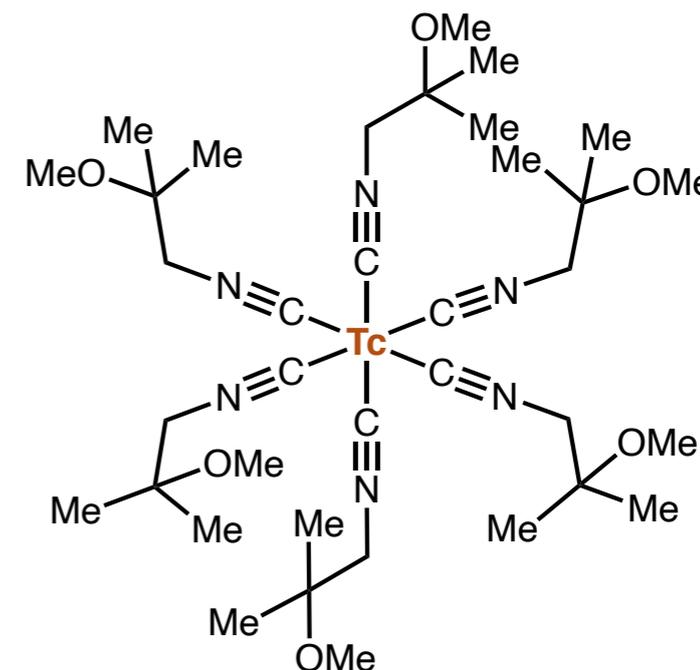
### $^{99m}\text{Tc}(\text{MDP})_2$

selectively absorbed by bone cells  
*localizes in bone cancers*



### $^{99m}\text{Tc}$ -exametazime

localizes in regions of impaired neurological activity  
*used in stroke diagnoses*



### $^{99m}\text{Tc}$ -HMIBI

cationic complex selectively absorbed by heart cells  
*used in cardiovascular diagnoses*

# LETTER

<https://doi.org/10.1038/s41586-019-1533-4>

## Energy of the $^{229}\text{Th}$ nuclear clock transition

Benedict Seiferle<sup>1\*</sup>, Lars von der Wense<sup>1</sup>, Pavlo V. Bilous<sup>2</sup>, Ines Amersdorffer<sup>1</sup>, Christoph Lemell<sup>3</sup>, Florian Libisch<sup>3</sup>, Simon Stellmer<sup>4</sup>, Thorsten Schumm<sup>5</sup>, Christoph E. Düllmann<sup>6,7,8</sup>, Adriana Pálffy<sup>2</sup> & Peter G. Thirolf<sup>1</sup>

# LETTER

<https://doi.org/10.1038/s41586-019-1542-3>

## X-ray pumping of the $^{229}\text{Th}$ nuclear clock isomer

Takahiko Masuda<sup>1</sup>, Akihiro Yoshimi<sup>1</sup>, Akira Fujieda<sup>1</sup>, Hiroyuki Fujimoto<sup>2</sup>, Hiromitsu Haba<sup>3</sup>, Hideaki Hara<sup>1</sup>, Takahiro Hiraki<sup>1</sup>, Hiroyuki Kaino<sup>1</sup>, Yoshitaka Kasamatsu<sup>4</sup>, Shinji Kitao<sup>5</sup>, Kenji Konashi<sup>6</sup>, Yuki Miyamoto<sup>1</sup>, Koichi Okai<sup>1</sup>, Sho Okubo<sup>1</sup>, Noboru Sasao<sup>1\*</sup>, Makoto Seto<sup>5</sup>, Thorsten Schumm<sup>7</sup>, Yudai Shigekawa<sup>4</sup>, Kenta Suzuki<sup>1</sup>, Simon Stellmer<sup>7,10</sup>, Kenji Tamasaku<sup>8</sup>, Satoshi Uetake<sup>1</sup>, Makoto Watanabe<sup>6</sup>, Tsukasa Watanabe<sup>2</sup>, Yuki Yasuda<sup>4</sup>, Atsushi Yamaguchi<sup>3</sup>, Yoshitaka Yoda<sup>9</sup>, Takuya Yokokita<sup>3</sup>, Motohiko Yoshimura<sup>1</sup> & Koji Yoshimura<sup>1\*</sup>

**$^{229m}\text{Th}$  - a low energy metastable isomer with applications for quantum computing and atomic clocks of unprecedented accuracy (nuclear transition vs. Cs electronic transition)**

## Notable Nuclear Isomers: $^{229m}\text{Th}$

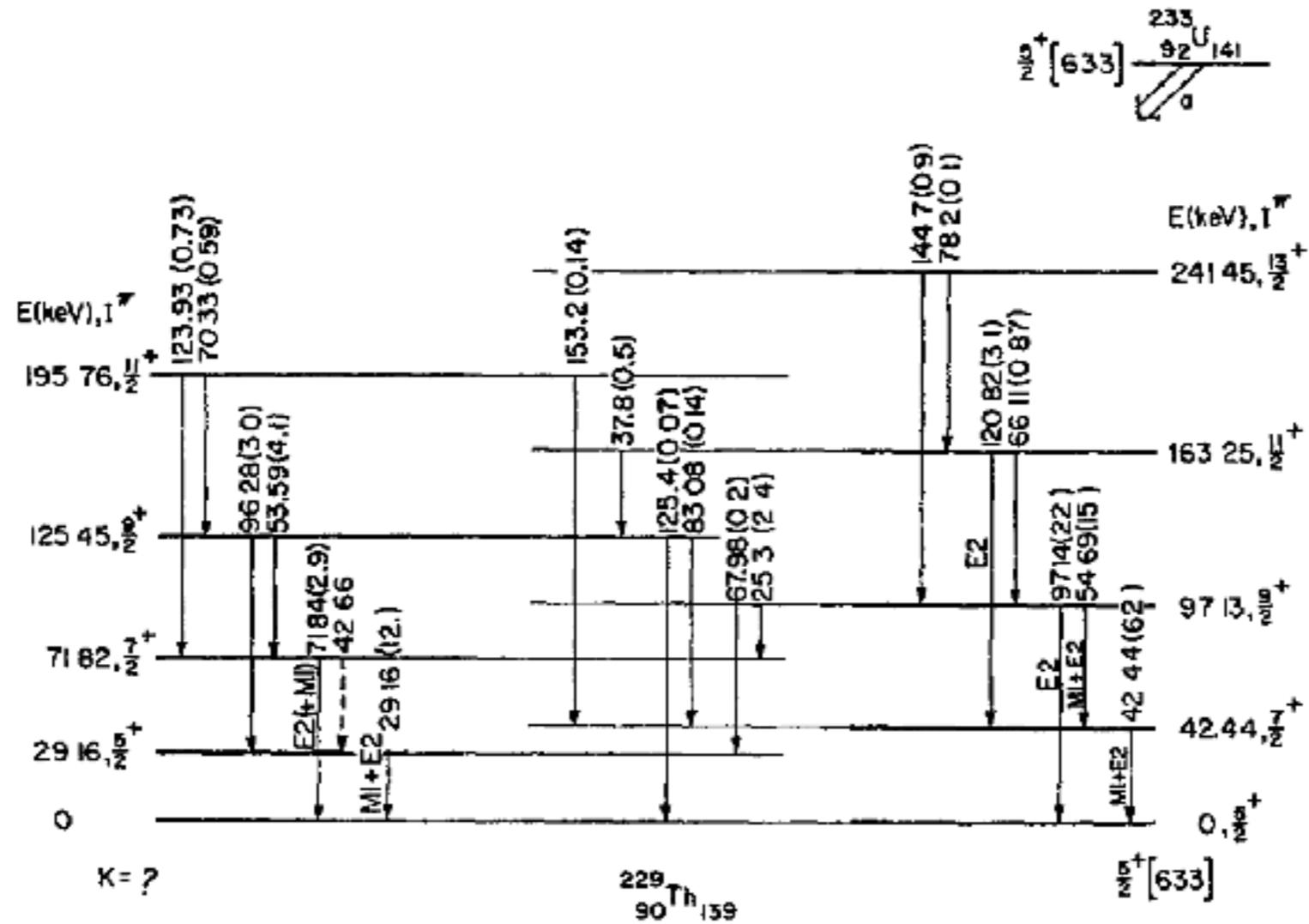


Fig. 6. Partial level scheme of  $^{229}\text{Th}$  showing the members of the two lowest lying positive-parity bands and their associated  $\gamma$ -ray transitions. Although the  $K$ -value of the band indicated at the left is shown as questionable, the reasoning presented in the text strongly suggests that this band is in fact built on the  $\frac{3}{2}^+$  [631] Nilsson state and that the  $I^\pi = \frac{3}{2}^+$  band head is located quite near to the ground state

The lowest of these bands is “shown from indirect evidence” to be within 0.1 keV of the ground state

## Notable Nuclear Isomers: $^{229m}\text{Th}$

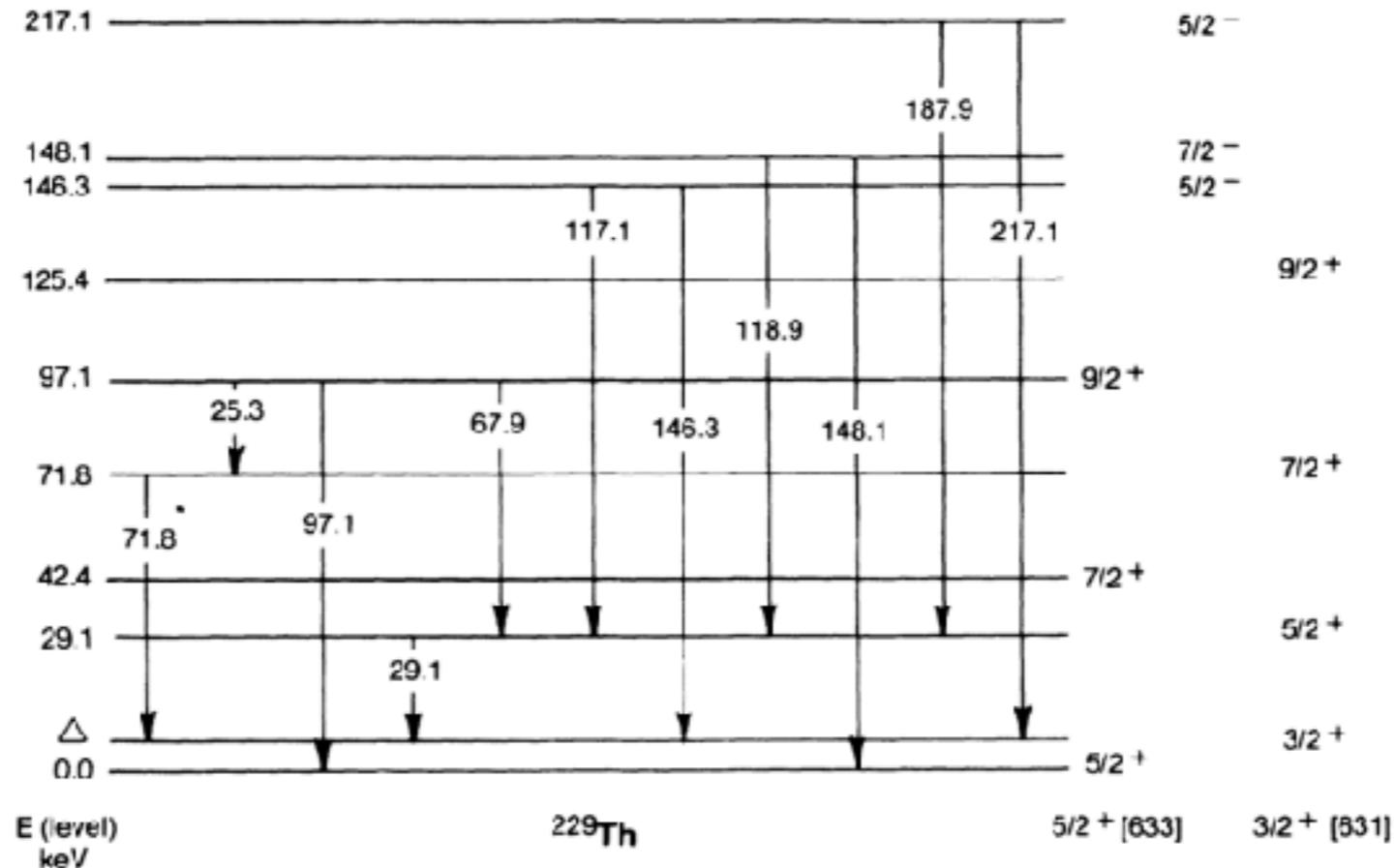


FIG. 1. Partial level scheme of  $^{229}\text{Th}$ , showing those  $\gamma$ -ray transitions whose energy values were used in determining the energy separation  $\Delta$  of the  $5/2^+$  [633] and  $3/2^+$  [631] bandheads.

3 separate indirect measurements afforded a band gap of:

$$\Delta_1 = -0.003 \pm 0.005 \text{ keV},$$

$$\Delta_2 = -0.001 \pm 0.006 \text{ keV},$$

$$\Delta_3 = +0.002 \pm 0.008 \text{ keV}.$$

The group concluded that the difference between the ground and excited isomeric state was  $<10 \text{ eV}$   
Instrumentation was no longer accurate enough to determine which state was the ground state

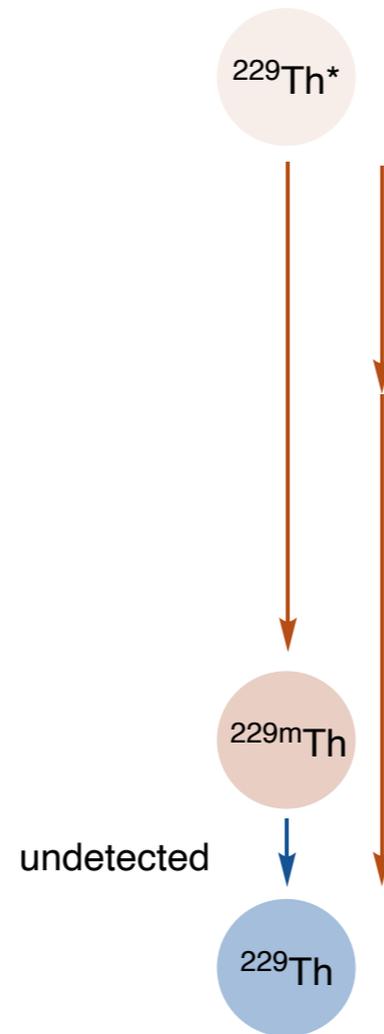
## Notable Nuclear Isomers: $^{229m}\text{Th}$

Subsequent studies throughout the early 2000's, enabled by improvements in gamma ray spectroscopy, determined the isomer to be  $7.8 \pm 0.5$  eV above the ground state



## Notable Nuclear Isomers: $^{229m}\text{Th}$

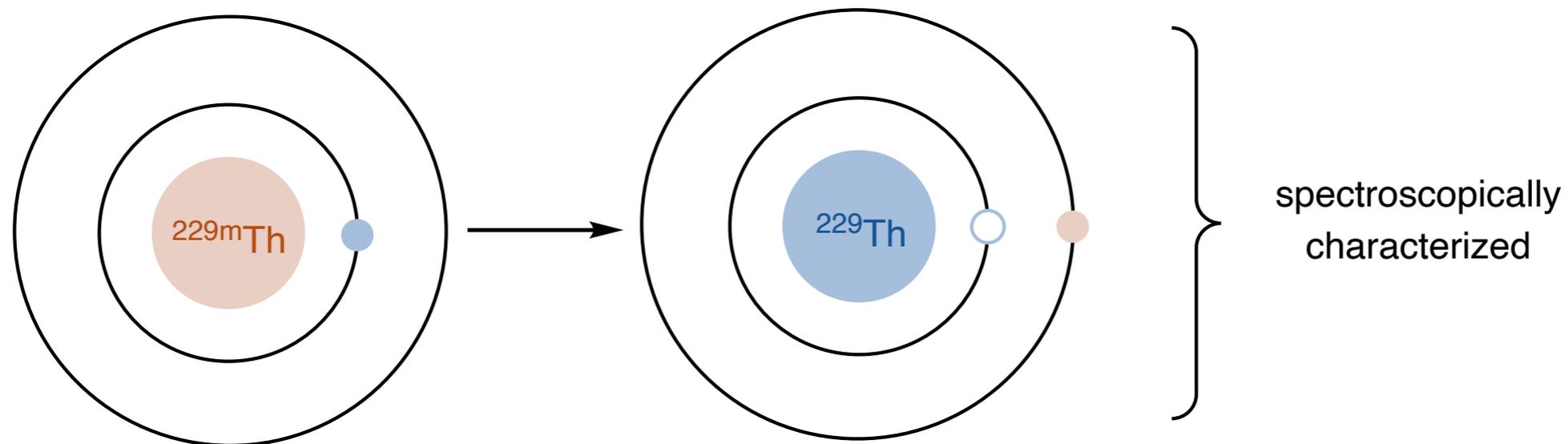
Subsequent studies throughout the early 2000's, enabled by improvements in gamma ray spectroscopy, determined the isomer to be  $7.8 \pm 0.5$  eV above the ground state



**No direct observation of the decay had yet been observed**

## Energy of the $^{229}\text{Th}$ nuclear clock transition

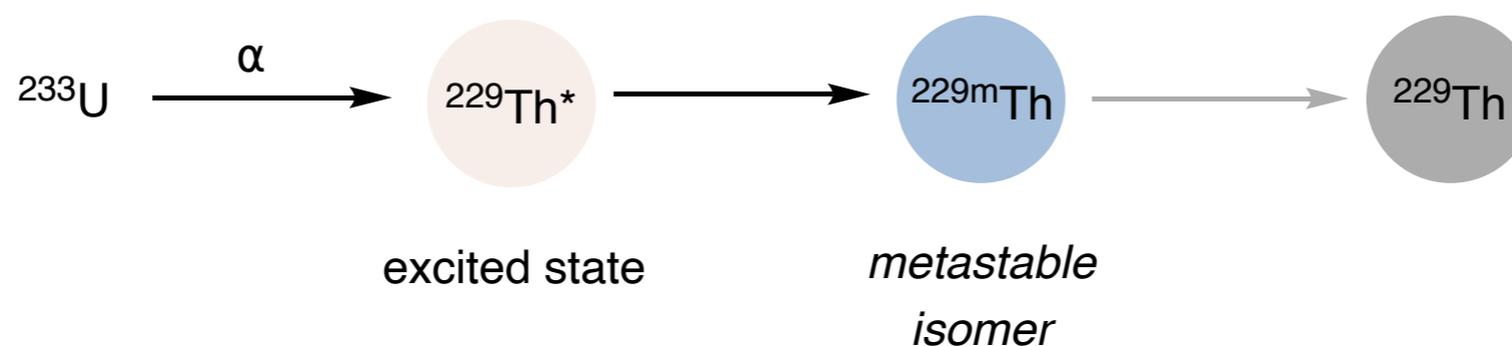
Benedict Seiferle<sup>1\*</sup>, Lars von der Wense<sup>1</sup>, Pavlo V. Bilous<sup>2</sup>, Ines Amersdorffer<sup>1</sup>, Christoph Lemell<sup>3</sup>, Florian Libisch<sup>3</sup>, Simon Stellmer<sup>4</sup>, Thorsten Schumm<sup>5</sup>, Christoph E. Düllmann<sup>6,7,8</sup>, Adriana Pálffy<sup>2</sup> & Peter G. Thirolf<sup>1</sup>



**Accurate calculation of the metastable state:  $149.7 \pm 3$  nm**

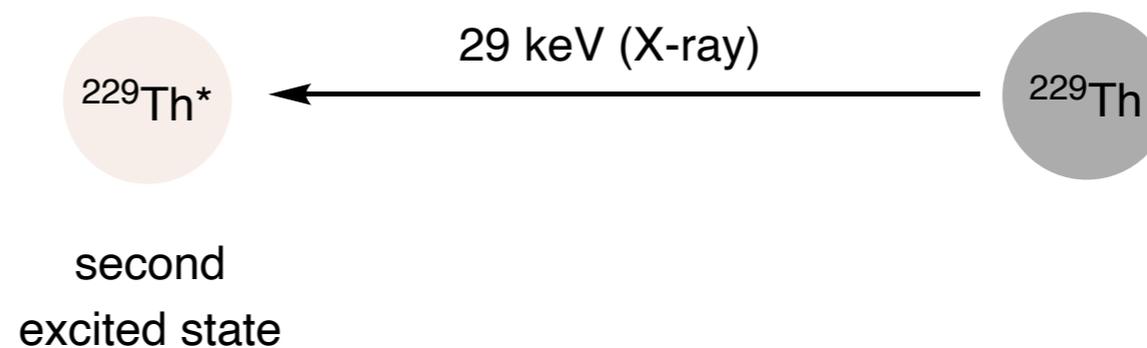
## X-ray pumping of the $^{229}\text{Th}$ nuclear clock isomer

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