



COMPLEXITY, SYMMETRY AND  
STRONG CORRELATIONS

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Solid State Physics 601  
Fall 2017

Phenomena Emerging  
from Complexity

# APPROACH TO COMPLEX PHENOMENA



reductionism



and emergence



## WHAT IS EMERGENCE ?

*Emergent phenomena in condensed-matter and materials physics are those that cannot be understood with models that treat the motions of the individual particles within the material independently. Instead, the essence of emergent phenomena lies in the complex interactions between many particles that result in the diverse behavior and often unpredictable collective motion of many particles.*

Condensed Matter and Materials Physics: The Science of the World Around Us, NAS, National Academies Press (2007).



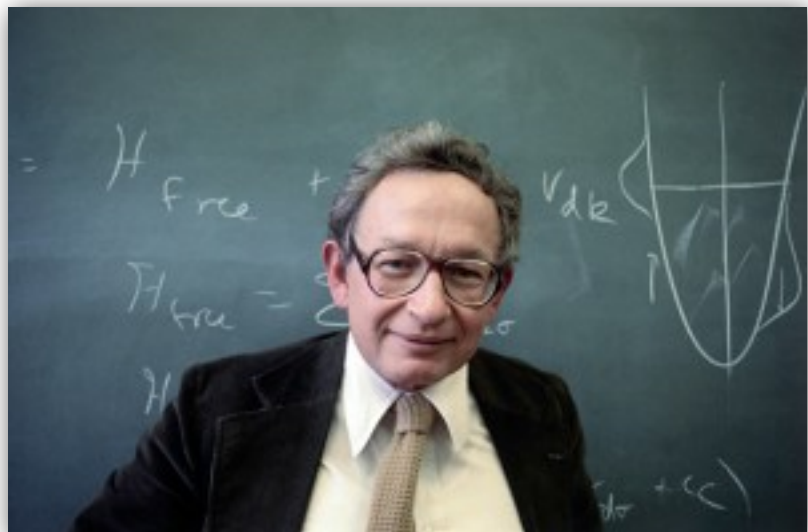
## More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson

## SCIENCE

4 August 1972, Volume 177, Number 4047



Nobel prize, 1977

## More is the Same; Phase Transitions and Mean Field Theories

Leo P. Kadanoff

J Stat Phys (2009) 137: 777–797

“Infinitely more is different.”



### *Summary of the paper: A dialog in Paris in 1920*

FITZGERALD: The rich are different from us.

HEMINGWAY: Yes, they have more money.

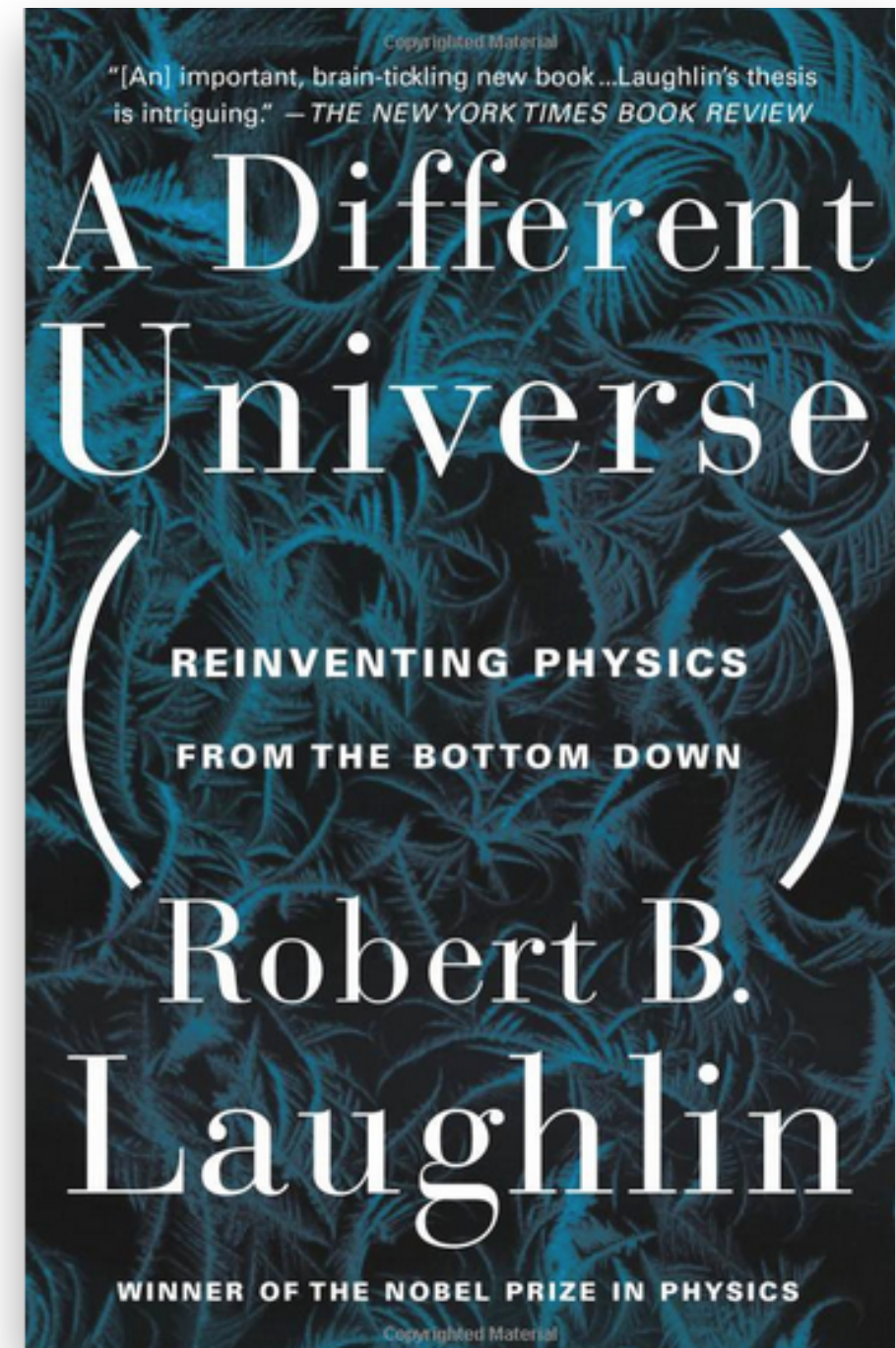
## 40 YEARS LATER ...



Robert B. Laughlin

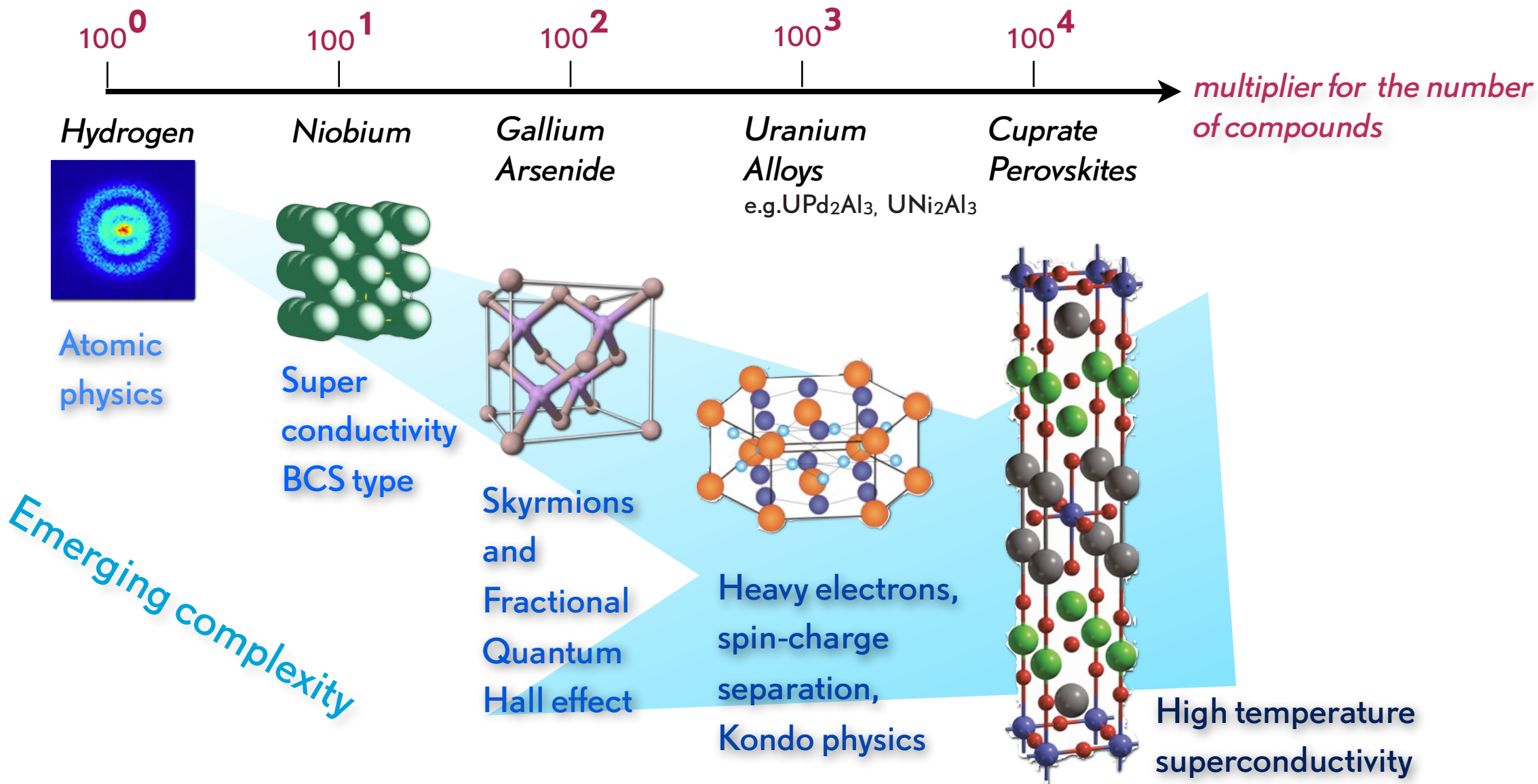
Nobel prize 1986

The low-energy excited quantum states of these systems [crystalline solids] are particles in exactly the same sense that the electron in the vacuum of quantum electrodynamics is a particle ... Yet they are not elementary, and, as in the case of sound, simply do not exist outside the context of the stable state of matter in which they live.





# COMPLEXITY IN SOLIDS





# Atomic Properties of the Elements

National Institute of Standards and Technology  
U.S. Department of Commerce

18  
VIII A

Physical Measurement

Standard

2  
II A

## delocalized p-electrons

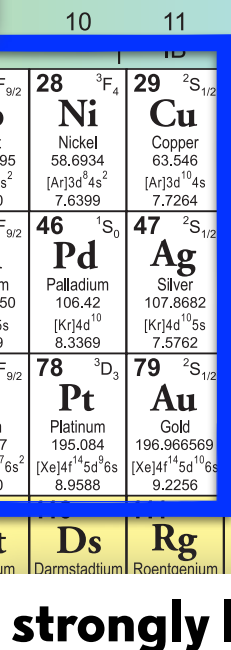
**Frequently used fundamental physical constants**

For the most accurate values of these and other constants, visit [physics.nist.gov/constants](http://physics.nist.gov/constants)  
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of <sup>133</sup>Cs

speed of light in vacuum	<i>c</i>	299 792 458	m s <sup>-1</sup>	(exact)
Planck constant	<i>h</i>	6.626 07 x 10 <sup>-34</sup>	J s	( <i>h</i> = <i>h</i> /2π)
elementary charge	<i>e</i>	1.602 177 x 10 <sup>-19</sup>	C	
electron mass	<i>m<sub>e</sub></i>	9.109 38 x 10 <sup>-31</sup>	kg	
	<i>m<sub>e</sub>c<sup>2</sup></i>	0.510 999	MeV	
proton mass	<i>m<sub>p</sub></i>	1.672 622 x 10 <sup>-27</sup>	kg	
fine-structure constant	<i>α</i>	1/137.035 999		
Rydberg constant	<i>R<sub>∞</sub></i>	10 973 731.569	m <sup>-1</sup>	
	<i>R<sub>∞</sub>c</i>	3.289 841 960 x 10 <sup>15</sup>	Hz	
Boltzmann constant				

- Solids
- Liquids
- Gases
- Artificially Prepared

## d-electrons



## strongly localized f-electrons

Group 1 IA	Group 2 IIA	Group 3 IIIB	Group 4 IVB	Group 5 VB	Group 6 VIB	Group 7 VIIB	Group 8 VIII	Group 9 VIII	Group 10 VIII	Group 11 IB	Group 12 IIB	Group 13 IIIA	Group 14 IV A	Group 15 VA	Group 16 VIA	Group 17 VIIA	Group 18 VIII A
1 <b>H</b> Hydrogen 1.008* 1s 13.5984	2 <b>He</b> Helium 4.002602 1s <sup>2</sup>	3 <b>Li</b> Lithium 6.94* 1s <sup>2</sup> 2s 5.3917	4 <b>Be</b> Beryllium 9.012182 1s <sup>2</sup> 2s <sup>2</sup> 9.3227	5 <b>B</b> Boron 10.81* 1s <sup>2</sup> 2s <sup>2</sup> 2p 8.2980	6 <b>C</b> Carbon 12.011* 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>2</sup> 11.2603	7 <b>N</b> Nitrogen 14.007* 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>3</sup> 14.5341	8 <b>O</b> Oxygen 15.999* 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>4</sup> 14.6184	9 <b>F</b> Fluorine 18.9984032 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>5</sup> 17.4228	10 <b>Ne</b> Neon 20.1797 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 21.5645	11 <b>Na</b> Sodium 22.98976928 [Ne]3s 5.1391	12 <b>Mg</b> Magnesium 24.3050 [Ne]3s <sup>2</sup> 7.6462	13 <b>Al</b> Aluminum 26.9815386 [Ne]3s <sup>2</sup> 3p 5.9858	14 <b>Si</b> Silicon 28.085* [Ne]3s <sup>2</sup> 3p <sup>2</sup> 8.1517	15 <b>P</b> Phosphorus 30.973762 [Ne]3s <sup>2</sup> 3p <sup>3</sup> 10.4867	16 <b>S</b> Sulfur 32.06* [Ne]3s <sup>2</sup> 3p <sup>4</sup> 10.3600	17 <b>Cl</b> Chlorine 35.45* [Ne]3s <sup>2</sup> 3p <sup>5</sup> 12.9676	18 <b>Ar</b> Argon 39.948 [Ne]3s <sup>2</sup> 3p <sup>6</sup> 15.7596
19 <b>K</b> Potassium 39.0983 [Ar]4s 4.3407	20 <b>Ca</b> Calcium 40.078 [Ar]4s <sup>2</sup> 6.1132	21 <b>Sc</b> Scandium 44.955912 [Ar]3d <sup>1</sup> 4s <sup>2</sup> 6.5615	22 <b>Ti</b> Titanium 47.867 [Ar]3d <sup>2</sup> 4s <sup>2</sup> 6.8281	23 <b>V</b> Vanadium 50.9415 [Ar]3d <sup>3</sup> 4s <sup>2</sup> 6.7462	24 <b>Cr</b> Chromium 51.9961 [Ar]3d <sup>5</sup> 4s 6.7665	25 <b>Mn</b> Manganese 54.938045 [Ar]3d <sup>5</sup> 4s <sup>2</sup> 7.4340	26 <b>Fe</b> Iron 55.845 [Ar]3d <sup>6</sup> 4s <sup>2</sup> 7.9025	27 <b>Co</b> Cobalt 58.933195 [Ar]3d <sup>7</sup> 4s <sup>2</sup> 7.8810	28 <b>Ni</b> Nickel 58.6934 [Ar]3d <sup>8</sup> 4s <sup>2</sup> 7.6399	29 <b>Cu</b> Copper 63.546 [Ar]3d <sup>10</sup> 4s 7.7264	30 <b>Zn</b> Zinc 65.38 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 9.3942	31 <b>Ga</b> Gallium 69.723 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p 5.9993	32 <b>Ge</b> Germanium 72.63 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>2</sup> 7.8994	33 <b>As</b> Arsenic 74.92160 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>3</sup> 9.7886	34 <b>Se</b> Selenium 78.96 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>4</sup> 9.7524	35 <b>Br</b> Bromine 79.904 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>5</sup> 11.8138	36 <b>Kr</b> Krypton 83.798 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>6</sup> 13.9996
37 <b>Rb</b> Rubidium 85.4678 [Kr]5s 4.1771	38 <b>Sr</b> Strontium 87.62 [Kr]5s <sup>2</sup> 5.6949	39 <b>Y</b> Yttrium 88.90585 [Kr]4d <sup>1</sup> 5s <sup>2</sup> 6.2173	40 <b>Zr</b> Zirconium 91.224 [Kr]4d <sup>2</sup> 5s <sup>2</sup> 6.6339	41 <b>Nb</b> Niobium 92.90638 [Kr]4d <sup>4</sup> 5s 6.7589	42 <b>Mo</b> Molybdenum 95.96 [Kr]4d <sup>5</sup> 5s 7.0924	43 <b>Tc</b> Technetium (98) [Kr]4d <sup>5</sup> 5s <sup>2</sup> 7.1194	44 <b>Ru</b> Ruthenium 101.07 [Kr]4d <sup>7</sup> 5s 7.3605	45 <b>Rh</b> Rhodium 102.90550 [Kr]4d <sup>8</sup> 5s 8.3369	46 <b>Pd</b> Palladium 106.42 [Kr]4d <sup>10</sup> 8.9938	47 <b>Ag</b> Silver 107.8682 [Kr]4d <sup>10</sup> 5s 7.5762	48 <b>Cd</b> Cadmium 112.411 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 8.9938	49 <b>In</b> Indium 114.818 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p 7.3439	50 <b>Sn</b> Tin 118.710 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>2</sup> 7.3439	51 <b>Sb</b> Antimony 121.760 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>3</sup> 8.6084	52 <b>Te</b> Tellurium 127.60 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>4</sup> 9.0097	53 <b>I</b> Iodine 126.90447 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup> 10.4513	54 <b>Xe</b> Xenon 131.293 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>6</sup> 12.1298
55 <b>Cs</b> Cesium 132.9054519 [Xe]6s 3.8939	56 <b>Ba</b> Barium 137.327 [Xe]6s <sup>2</sup> 5.2117	57 <b>La</b> Lanthanum 138.90547 [Xe]5d <sup>1</sup> 6s <sup>2</sup> 5.5769	58 <b>Ce</b> Cerium 140.116 [Xe]4f <sup>1</sup> 5d <sup>1</sup> 6s <sup>2</sup> 5.5386	59 <b>Pr</b> Praseodymium 140.90765 [Xe]4f <sup>3</sup> 6s <sup>2</sup> 5.473	60 <b>Nd</b> Neodymium 144.242 [Xe]4f <sup>4</sup> 6s <sup>2</sup> 5.5250	61 <b>Pm</b> Promethium (145) [Xe]4f <sup>5</sup> 6s <sup>2</sup> 5.582	62 <b>Sm</b> Samarium 150.36 [Xe]4f <sup>6</sup> 6s <sup>2</sup> 5.6437	63 <b>Eu</b> Europium 151.964 [Xe]4f <sup>7</sup> 6s <sup>2</sup> 5.6704	64 <b>Gd</b> Gadolinium 157.25 [Xe]4f <sup>7</sup> 5d <sup>1</sup> 6s <sup>2</sup> 6.1498	65 <b>Tb</b> Terbium 158.92535 [Xe]4f <sup>9</sup> 6s <sup>2</sup> 5.8638	66 <b>Dy</b> Dysprosium 162.500 [Xe]4f <sup>10</sup> 6s <sup>2</sup> 5.9391	67 <b>Ho</b> Holmium 164.93032 [Xe]4f <sup>11</sup> 6s <sup>2</sup> 6.0215	68 <b>Er</b> Erbium 167.259 [Xe]4f <sup>12</sup> 6s <sup>2</sup> 6.1077	69 <b>Tm</b> Thulium 168.93421 [Xe]4f <sup>13</sup> 6s <sup>2</sup> 6.1843	70 <b>Yb</b> Ytterbium 173.054 [Xe]4f <sup>14</sup> 6s <sup>2</sup> 6.2542	71 <b>Lu</b> Lutetium 174.9668 [Xe]4f <sup>14</sup> 5d <sup>1</sup> 6s <sup>2</sup> 5.4259	
87 <b>Fr</b> Francium (223) [Rn]7s 4.0727	88 <b>Ra</b> Radium (226) [Rn]7s <sup>2</sup> 5.2784	89 <b>Ac</b> Actinium (227) [Rn]6d <sup>1</sup> 7s <sup>2</sup> 5.3802	90 <b>Th</b> Thorium 232.03806 [Rn]6d <sup>2</sup> 7s <sup>2</sup> 6.3067	91 <b>Pa</b> Protactinium 231.03588 [Rn]5f <sup>1</sup> 6d <sup>1</sup> 7s <sup>2</sup> 5.89	92 <b>U</b> Uranium 238.02891 [Rn]5f <sup>3</sup> 6d <sup>1</sup> 7s <sup>2</sup> 6.1941	93 <b>Np</b> Neptunium (237) [Rn]5f <sup>4</sup> 6d <sup>1</sup> 7s <sup>2</sup> 6.2655	94 <b>Pu</b> Plutonium (244) [Rn]5f <sup>6</sup> 7s <sup>2</sup> 6.0258	95 <b>Am</b> Americium (243) [Rn]5f <sup>7</sup> 7s <sup>2</sup> 5.9738	96 <b>Cm</b> Curium (247) [Rn]5f <sup>8</sup> 6d <sup>1</sup> 7s <sup>2</sup> 5.9914	97 <b>Bk</b> Berkelium (247) [Rn]5f <sup>9</sup> 7s <sup>2</sup> 6.1978	98 <b>Cf</b> Californium (251) [Rn]5f <sup>10</sup> 7s <sup>2</sup> 6.2817	99 <b>Es</b> Einsteinium (252) [Rn]5f <sup>11</sup> 7s <sup>2</sup> 6.3676	100 <b>Fm</b> Fermium (257) [Rn]5f <sup>12</sup> 7s <sup>2</sup> 6.50	101 <b>Md</b> Mendelevium (258) [Rn]5f <sup>13</sup> 7s <sup>2</sup> 6.58	102 <b>No</b> Nobelium (259) [Rn]5f <sup>14</sup> 7s <sup>2</sup> 6.65	103 <b>Lr</b> Lawrencium (262) [Rn]5f <sup>14</sup> 7p 4.90	

Atomic Number: 58  
Ground-state Level: 1G<sub>4</sub><sup>o</sup>  
Symbol: **Ce**  
Name: Cerium  
Standard Atomic Weight: 140.116  
Ground-state Configuration: [Xe]4f<sup>1</sup>5d<sup>1</sup>6s<sup>2</sup>  
Ionization Energy (eV): 5.5386

A masterplan for designing complex materials



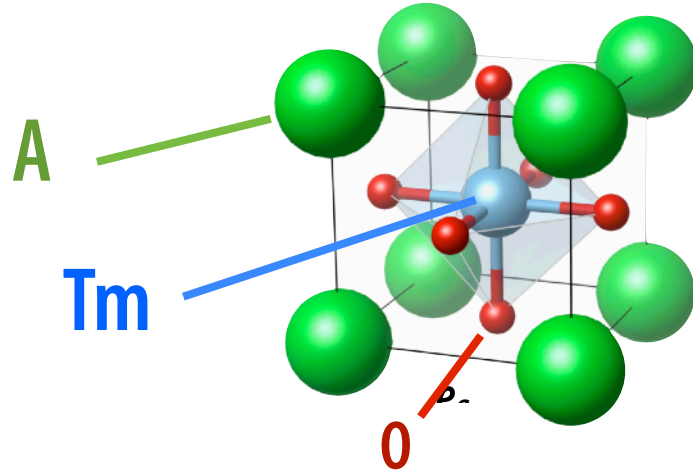


# PEROVSKITE COMPLEX OXIDES

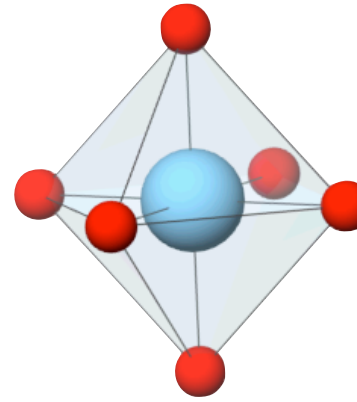
$A = \text{La, Ce, Pr} \dots$   $Tm = \text{Fe, Ru, Ir} \dots$

e.g.  $\text{CaTiO}_3$ ,  $\text{NdNiO}_3$ ,  $\text{SrMnO}_3$

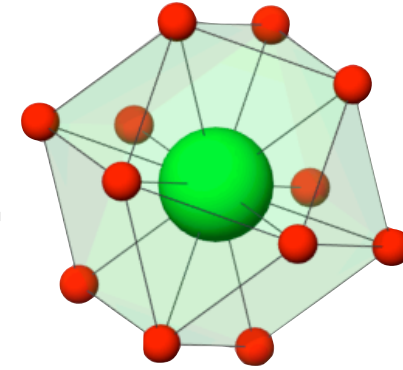
$AMO_3$  perovskite unit cell



=



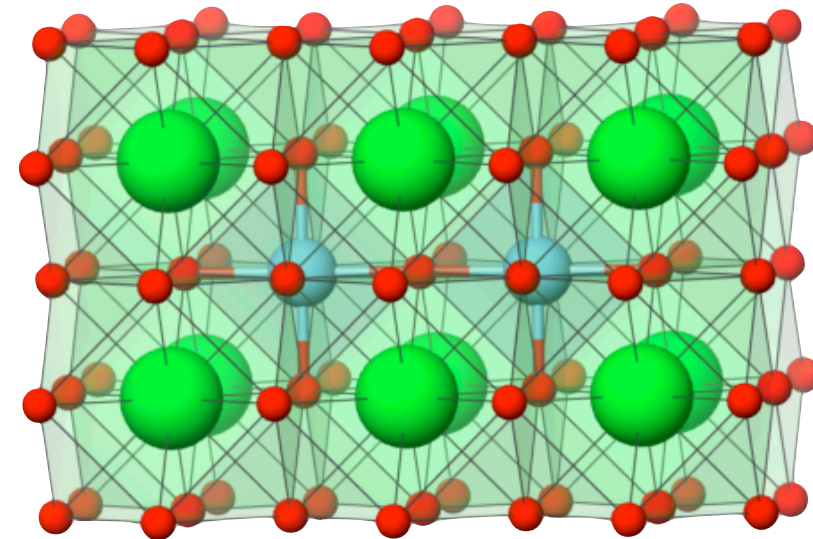
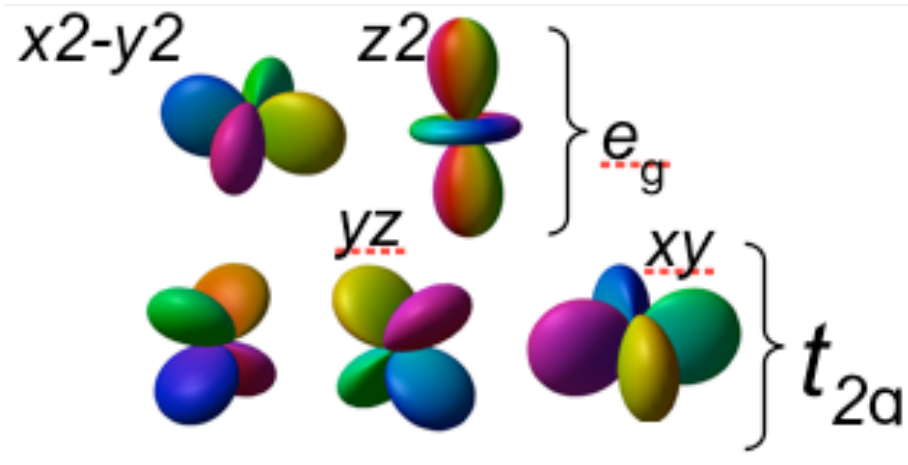
+



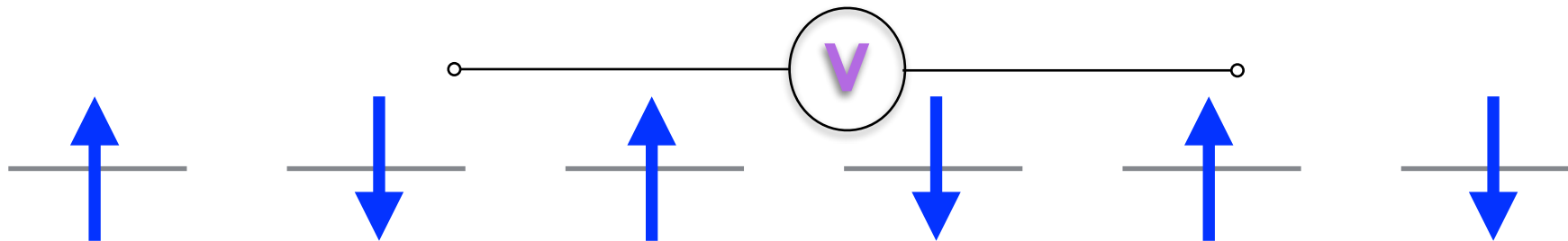
$MO_6$   
rigid

$AO_{12}$   
soft

5 distinct atomic orbital shapes on  $M$



# STRONG CORRELATIONS - MOTT INSULATORS

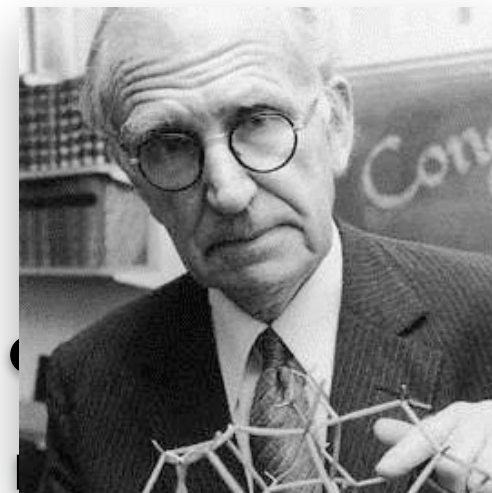


Electron counting loses coulomb energy,  $U$

$\text{La}_2\text{CuO}_4$ : 2 La (57x2)+Cu (29) + 4 O (4x8)=175 electrons

but  $\text{La}_2\text{CuO}_4$  is a strong insulator!

gains kinetic energy,  $t$



Nevill Francis Mott

Nobel prize 1977

**even**  
insulator

For  $U \gg t$  electrons localize: **Mott insulator**

Small  $U/t$

Increasing  $U/t$

Large  $U/t$

Metal



Insulator

# COMPLEXITY IN CORRELATED MATERIALS

local entanglement of ***lattice, charge, spin,*** and ***orbital degrees of freedom*** defines multiple *closely spaced energy landscape* with meta-stable ground states

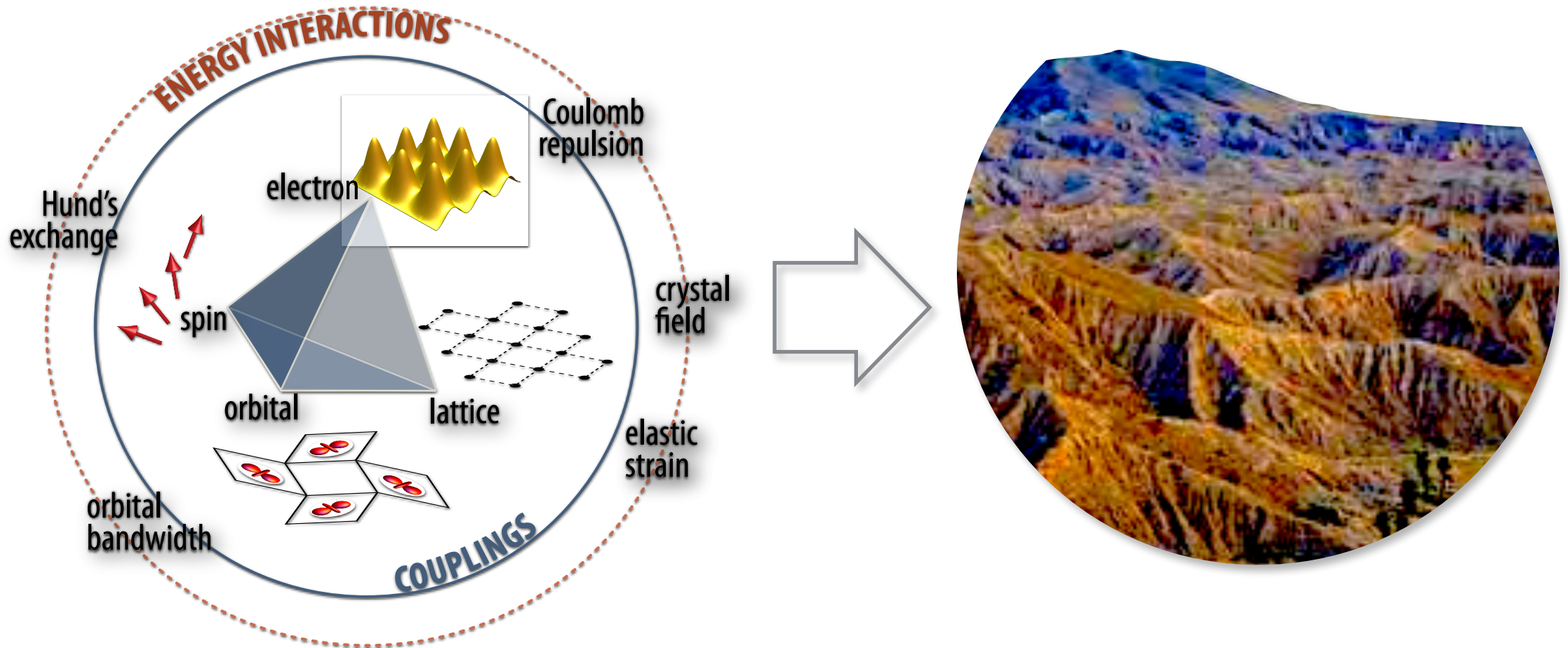


Fig. J.M. Rondinelli and N.A. Spaldin, *Adv. Mater.* (2011)

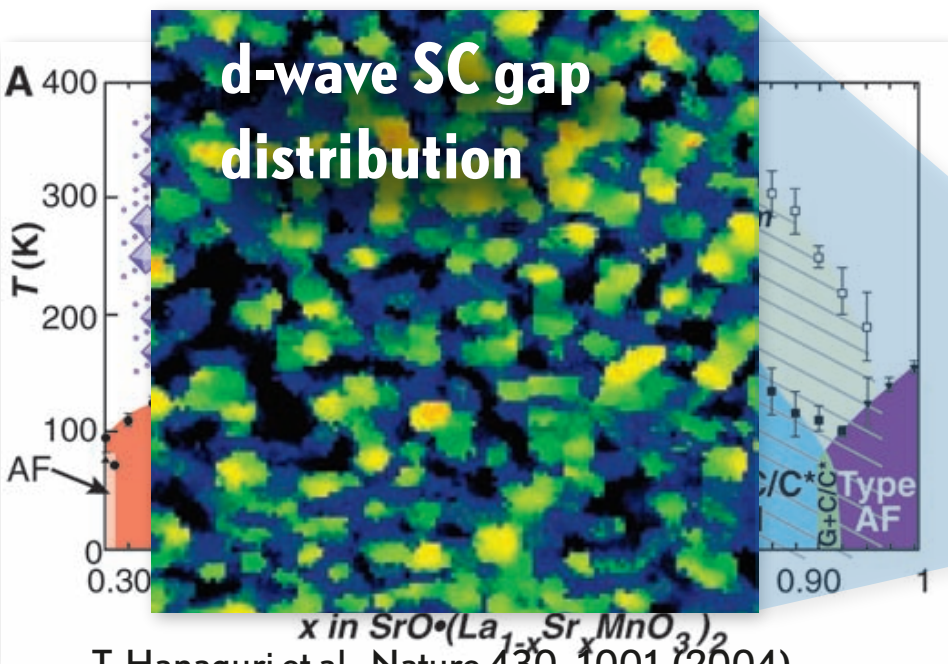


# EMERGING COMPLEXITY FROM STRONG CORRELATIONS

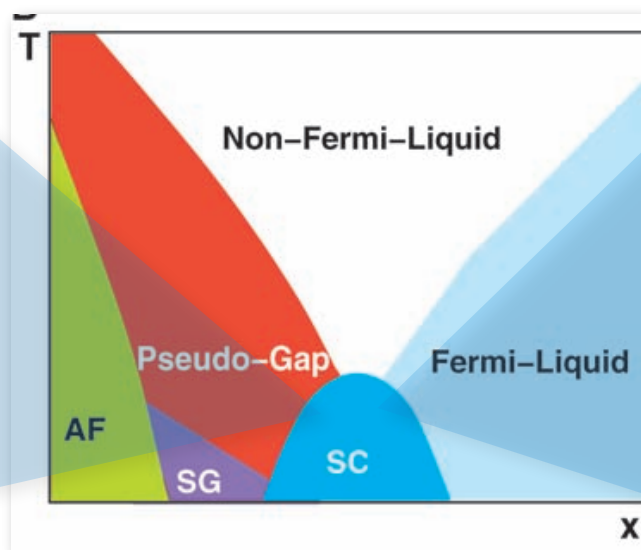
## Complexity in Strongly Correlated Electronic Systems

Elbio Dagotto

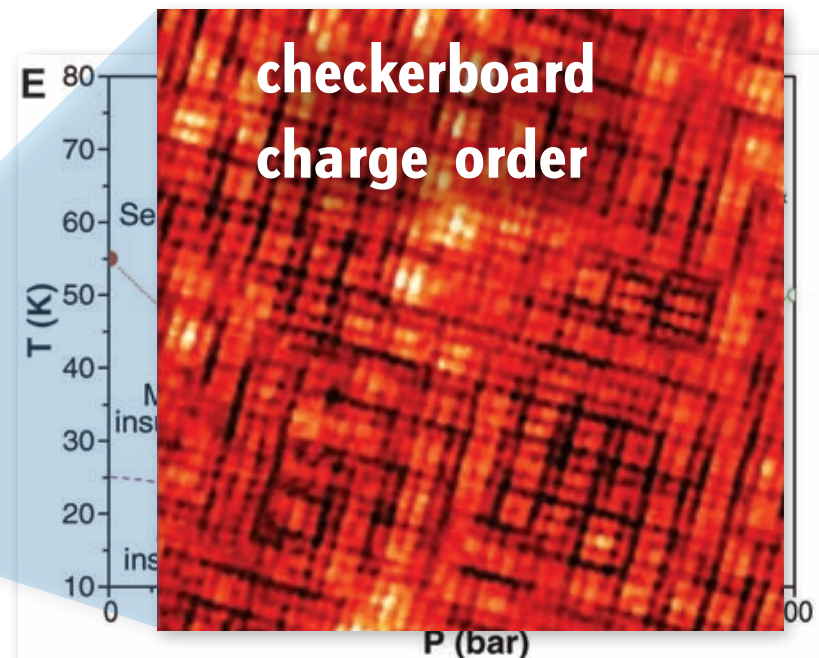
SCIENCE VOL 309 8 JULY 2005



Colossal magnetoresistance (CMR) manganites



High  $T_c$  superconducting cuprates e.g.  $YBa_2Cu_3O_{7-x}$



Organic 1D salts e.g.  $k-(BEDT-TTF)_2Cu[N(CN)_2]Cl$  (2004)

Exciting physics but hard to realize in bulk materials

# Broken Symmetry and Emerging Phases



# SIGNS OF EMERGENT BEHAVIOR

Phase transitions usually involve *symmetry breaking*—a change in the symmetry of the constituents. For example, the molecules in a liquid are randomly

Condensed Matter and Materials Physics: The Science of the World Around Us, National Academies Press (2007).



# SYMMETRY IN SPACE - INVERSION, ROTATION, TRANSLATION

Most fundamental idea - central to many modern sciences

In antiquity synonymous with harmony and beauty  
/ inversion symmetry, translational symmetry /



Symmetry in art  
/ rotational symmetry /



Symmetry in biology



# SYMMETRY IN TIME OR TIME INVERSION



CRAB CANON JSB

CRAB CANON JSB

The image shows two systems of musical notation for the Crab Canon. Each system consists of two staves. The top system is labeled 'CRAB CANON JSB' and the bottom system is also labeled 'CRAB CANON JSB'. The notation is in G minor, 3/4 time, and features a complex, interlocking melodic pattern. The bottom system includes a '+' symbol above the first measure of the upper staff, indicating a specific rhythmic or melodic feature.



The image shows two systems of musical notation for the Crab Canon. Each system consists of two staves. The notation is in G minor, 3/4 time, and features a complex, interlocking melodic pattern. The bottom system includes a '+' symbol above the first measure of the upper staff, indicating a specific rhythmic or melodic feature.

A canon "Quaerendo invenietis" based on **retrogression**

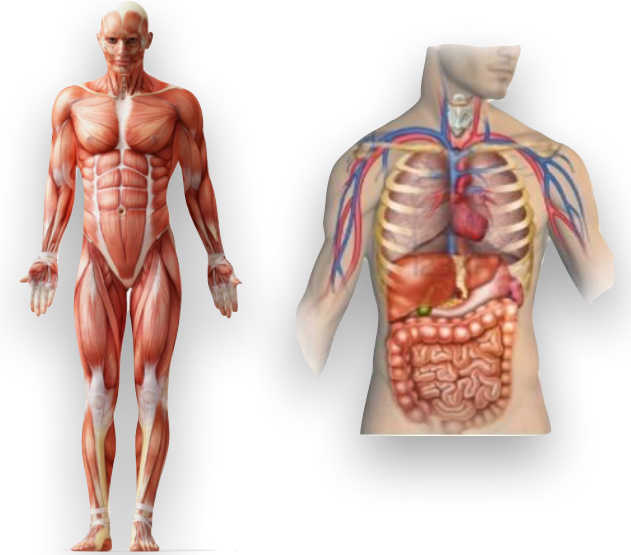
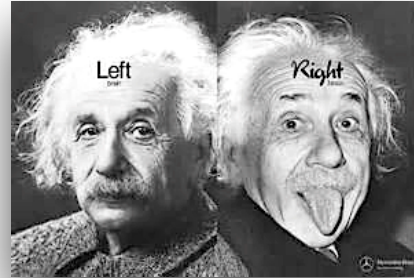
J.S. Bach, The Musical Offering, BWV 1079



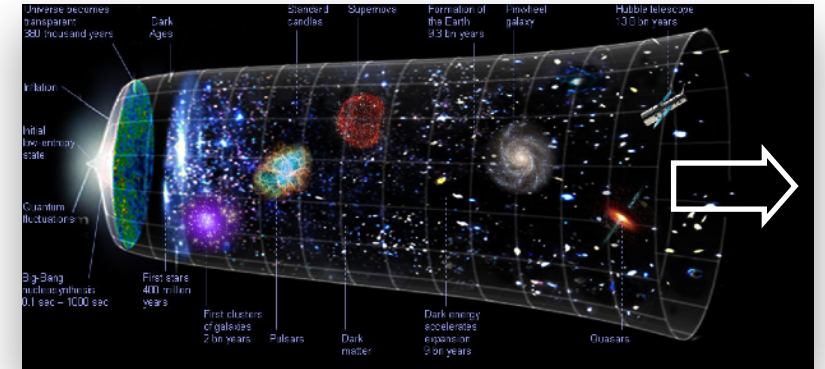
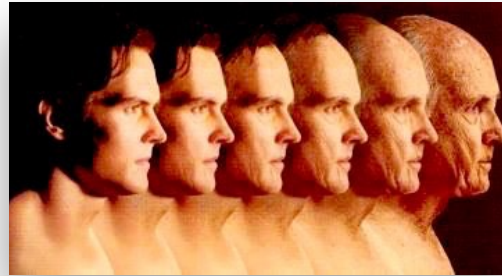


# BROKEN SYMMETRY

Left vs. Right

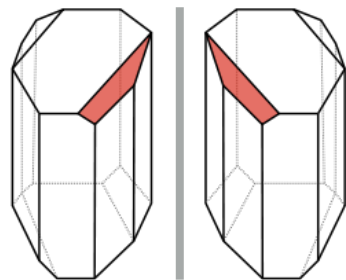
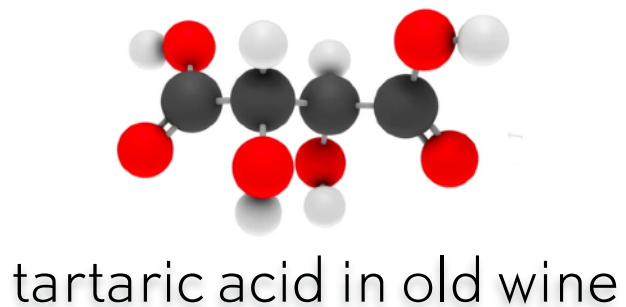


Arrow of time - past vs. future

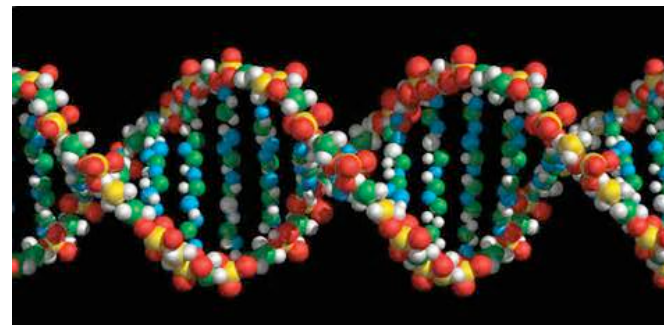


# CHIRALITY OR BROKEN SYMMETRY OF LIFE

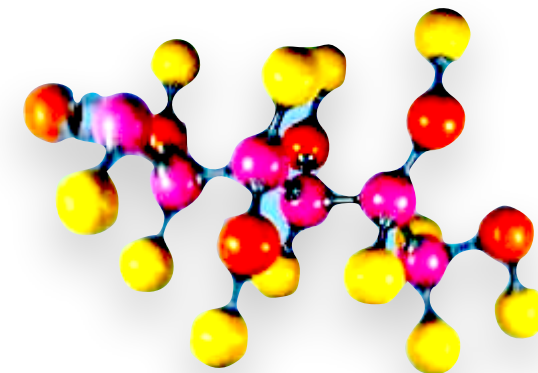
molecules of life are chiral !



DNA



sugars



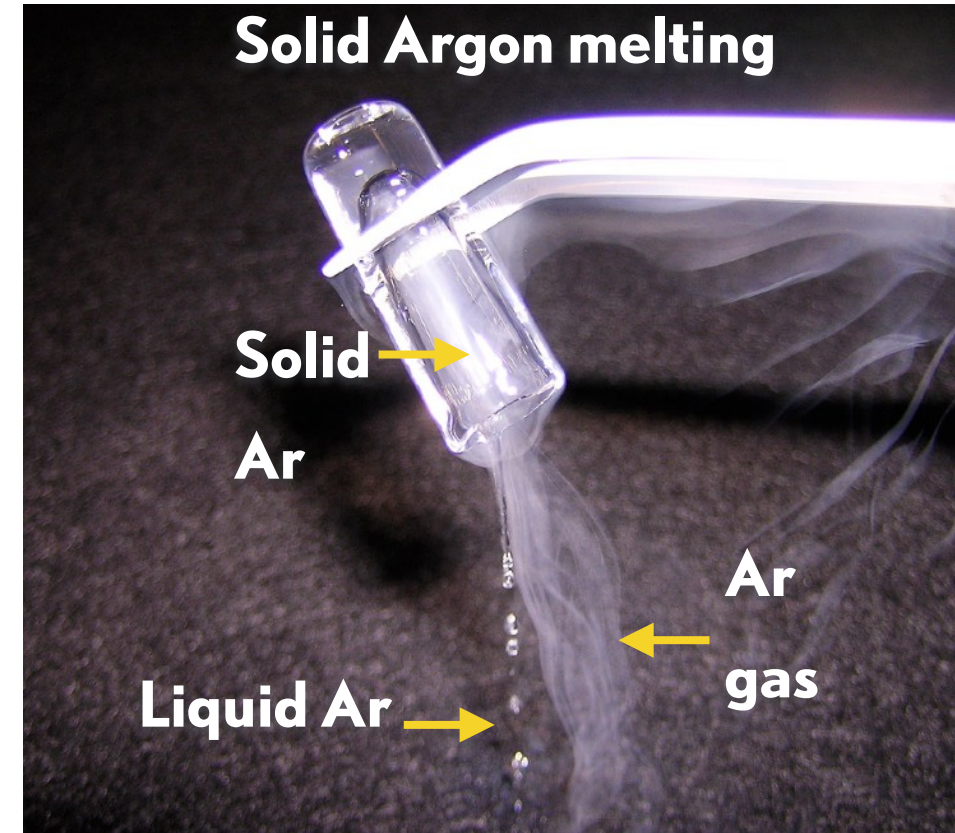
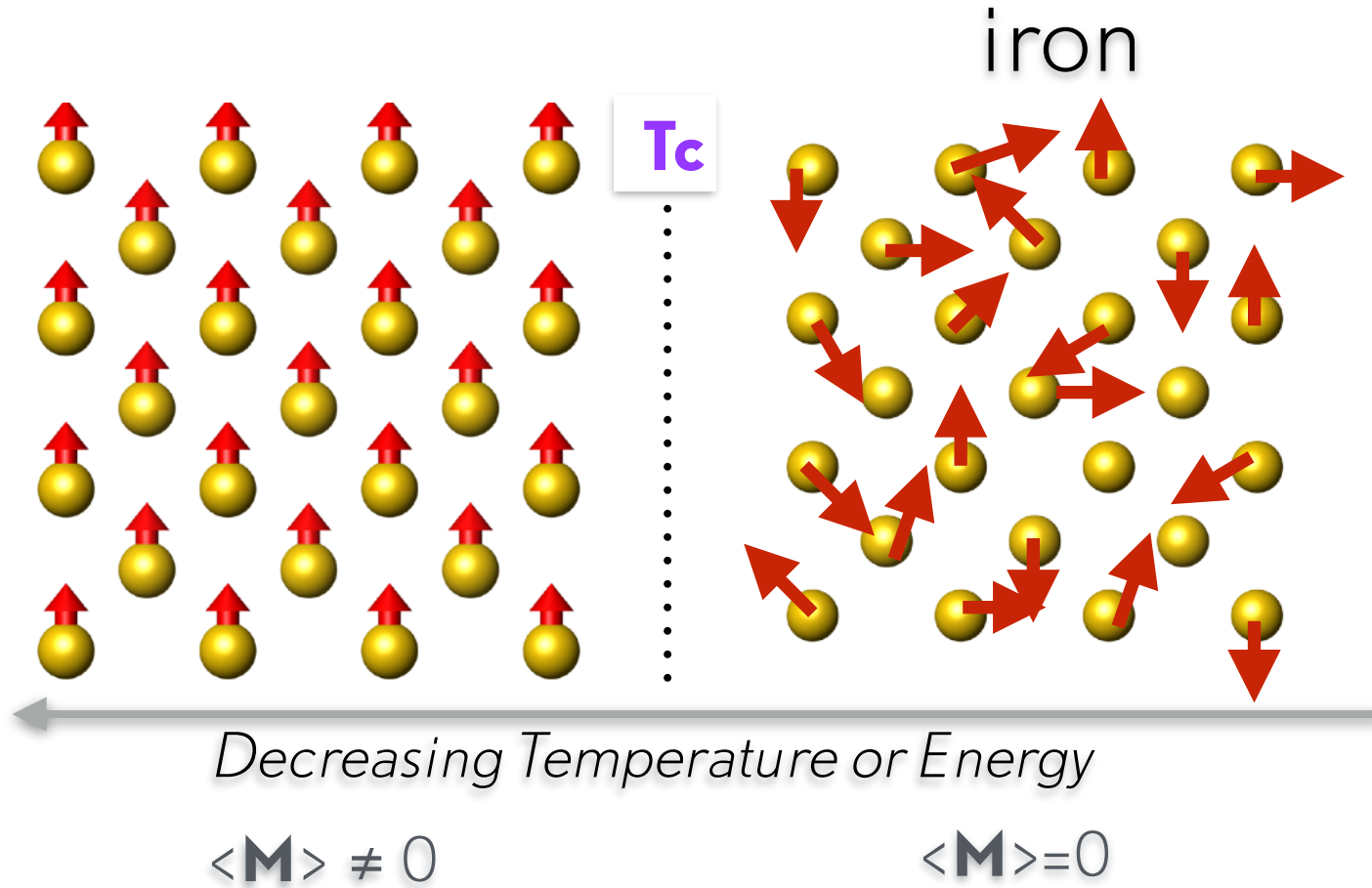
Louis Pasteur  
1822-1895

"I am inclined to think that life, as manifested to us, must be a function of the dissymmetry of the universe and of the consequences it produces.... Life is dominated by dissymmetrical actions. I can even foresee that all living species are primordially, in their structure, in their external forms, functions of cosmic dissymmetry."

c.1850



# BROKEN SYMMETRY = EMERGENCE OF A NEW PHASE



A tri-critical point of Ar



# (BROKEN) SYMMETRY AND ORDER PARAMETER

Temperature or Energy ↑

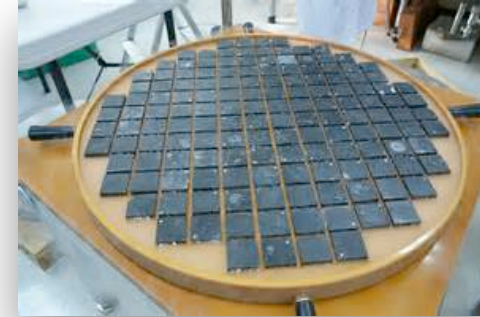
liquid



metal



magnetic insulator



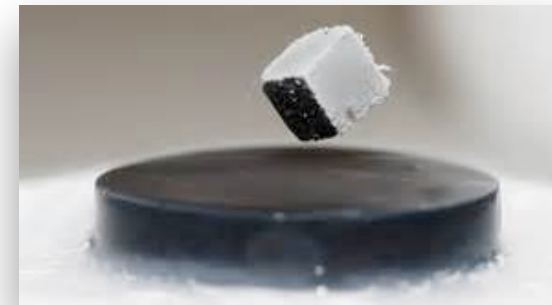
critical temperature  $T_c$



solid



insulator



superconductor

disordered phase  
**higher** symmetry

ordered phase  
**lower** symmetry

**Broken symmetry** means the appearance of an ordered phase with a **non-zero order parameter**

## WHERE ARE THE NEW PHASES OF MATTER?



Lev Landau  
Nobel prize  
1962

*Landau “recipes”* for getting new phases and states:

The sudden **disappearance of a certain symmetry** in the high-symmetry phase leads to the **occurrence of a phase transition** into **a new phase** with lower symmetry.

**If we assume control over symmetry breaking, we may end up with new designer phases**