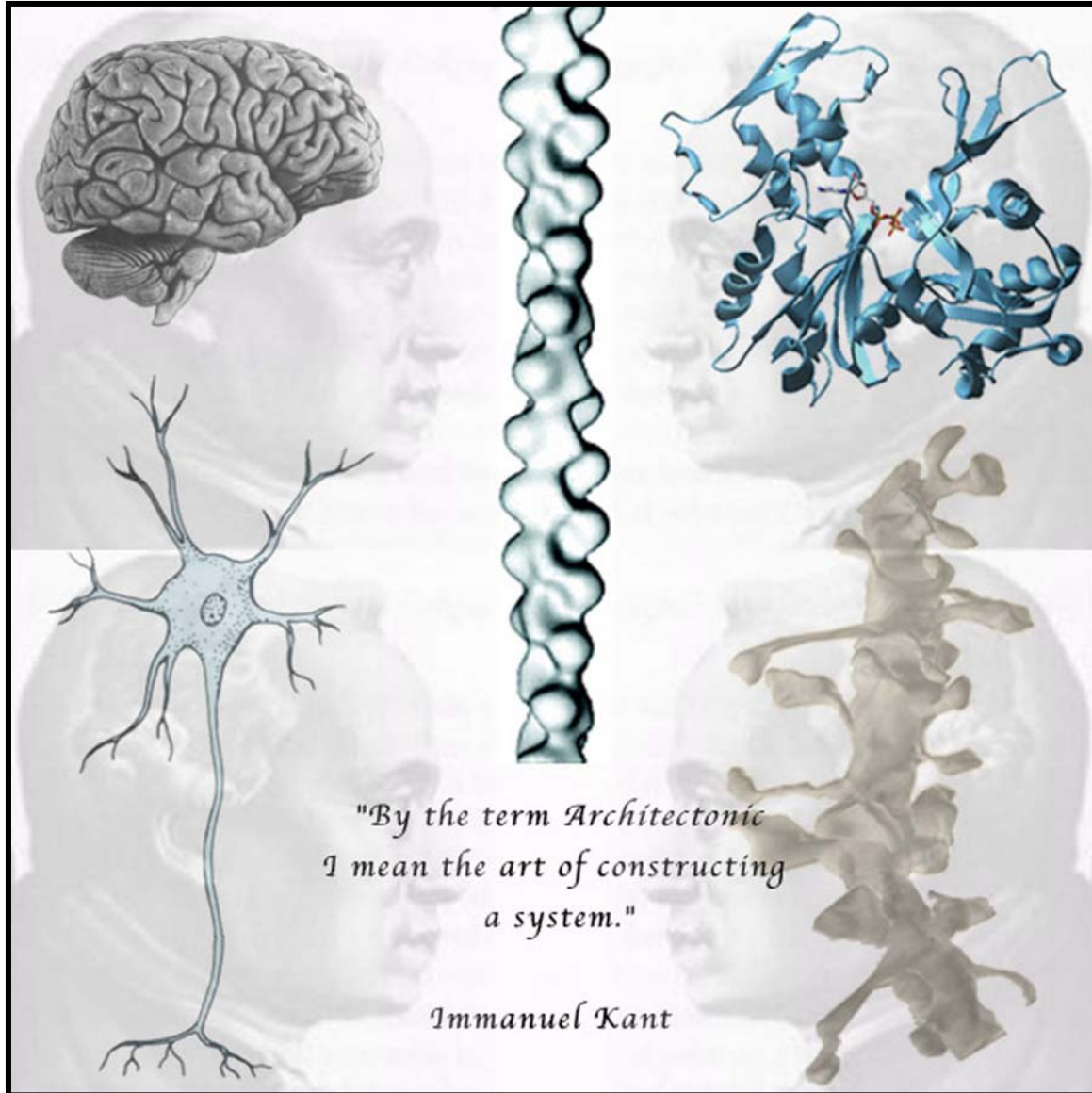


# The Origins of Life: An Architectonic Perspective

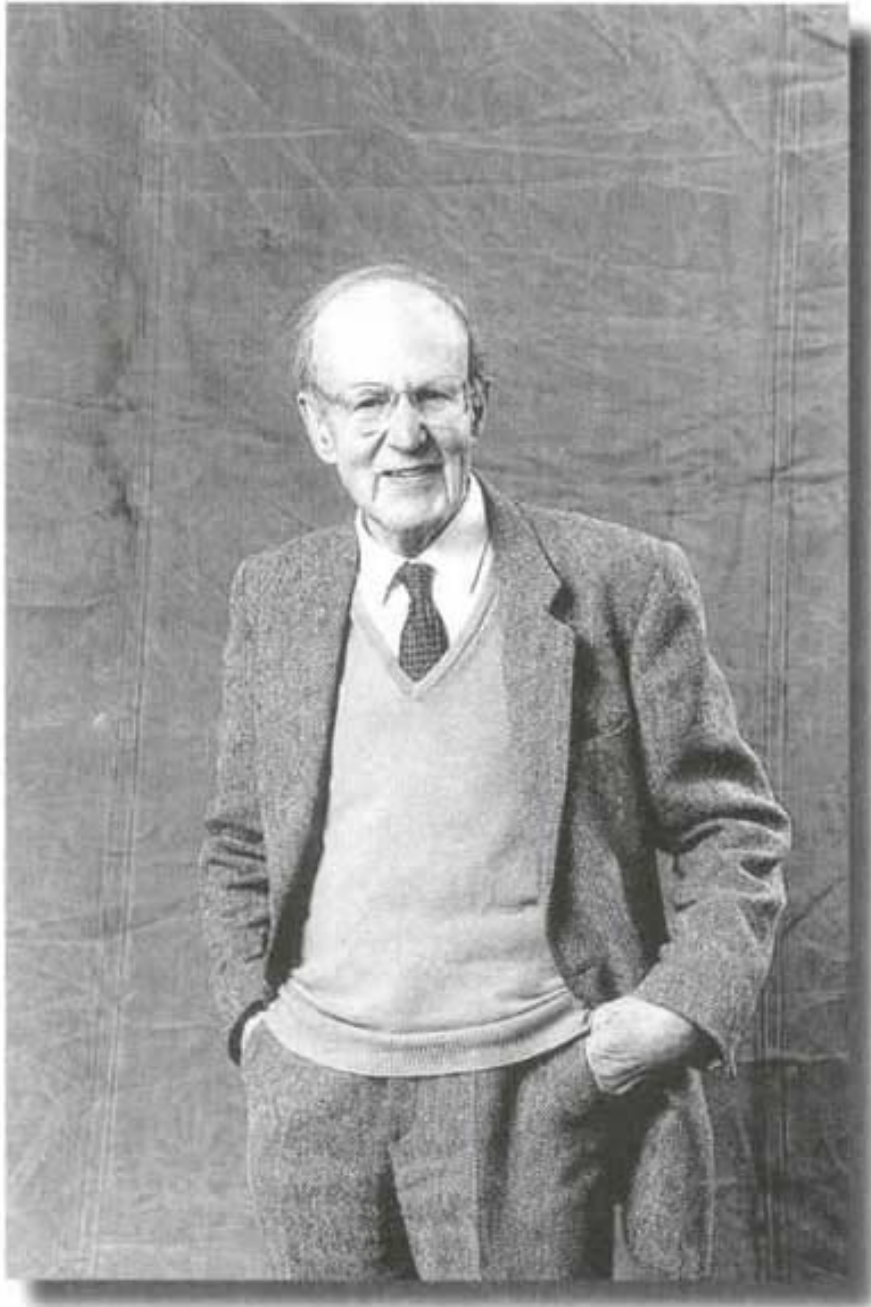
28 March 2007

Clarence E. Schutt  
Princeton University



"By the term *Architectonic*  
I mean the art of constructing  
a system."

*Immanuel Kant*



# Dedicated to Max Perutz

(1914 - 2002)

QuickTime™ and a  
TIFF (Uncompressed) decompressor  
are needed to see this picture.

# Outline of Today's Presentation

1. Two Architectonic Principles from Schrödinger:

-*Negentropy*

-*The Aperiodic Crystal*

2. Order from order: Light, Crystals, Life

3. Order from disorder: Proteins, Viruses

4. The Third Architectonic Principle: muscle contraction

# Schrödinger: “Is Life Based on the Laws of Physics?”

“What I wish to make clear ... is ...that from all that we have learnt about the structure of living matter, we must be prepared to find it working in a manner that cannot be reduced to the ordinary laws of physics. And that not on the ground that there is any ‘new force’ but ... because the *construction* is different from anything we have yet tested in the physical laboratory.”

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TIFF (Uncompressed) decompressor  
are needed to see this picture.

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TIFF (Uncompressed) decompressor  
are needed to see this picture.

# Michael Polanyi: “Life’s Irreducible Structure (Science, 1968)”

“In this light the organism is shown to be, like a machine, a system which works according to two different principles: its *structure* serves as a *boundary condition* harnessing physical-chemical processes by which its organs perform their functions.”

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TIFF (Uncompressed) decompressor  
are needed to see this picture.

1891-1976

QuickTime™ and a  
TIFF (Uncompressed) decompressor  
are needed to see this picture.

The electric motor places constraints on the  
movement of the electrons

# Two ideas from Schrödinger's book, 'What Is Life?'

The order in living systems on Earth is only in apparent violation of the second law of thermodynamics. Life feeds on 'negative entropy'.

$$\Delta S_{\text{universe}} \geq 0$$

The stability of genes over the span of lifetimes suggests that they are *a*periodic crystals, coding in their quantum states the plan of the organism.

# Max Perutz on ‘What Is Life?’

“The apparent contradictions between life and the statistical laws of physics can be resolved by invoking a science largely ignored by Schrödinger. That science is chemistry.”

$$\Delta G_{\text{life}} = \Delta H_{\text{life}} - T\Delta S_{\text{life}} \leq 0$$

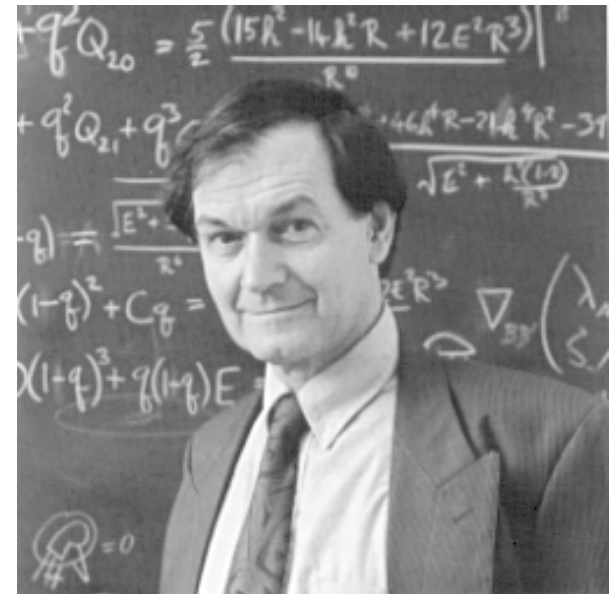
“Given a source of free energy, a well-ordered configuration of atoms in a single molecule of an enzyme catalyst can direct the formation of an ordered stereospecific compound ... thus creating *order from disorder* at the ultimate expense of solar energy.”

“Physics and the Riddle of Life”, Nature (326), 1987



# Roger Penrose: The Entropy of Light

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TIFF (Uncompressed) decompressor  
are needed to see this picture.



$$\Delta S_{\text{light}} = S_{\text{infrared}} - S_{\text{ultraviolet}} \geq 0$$

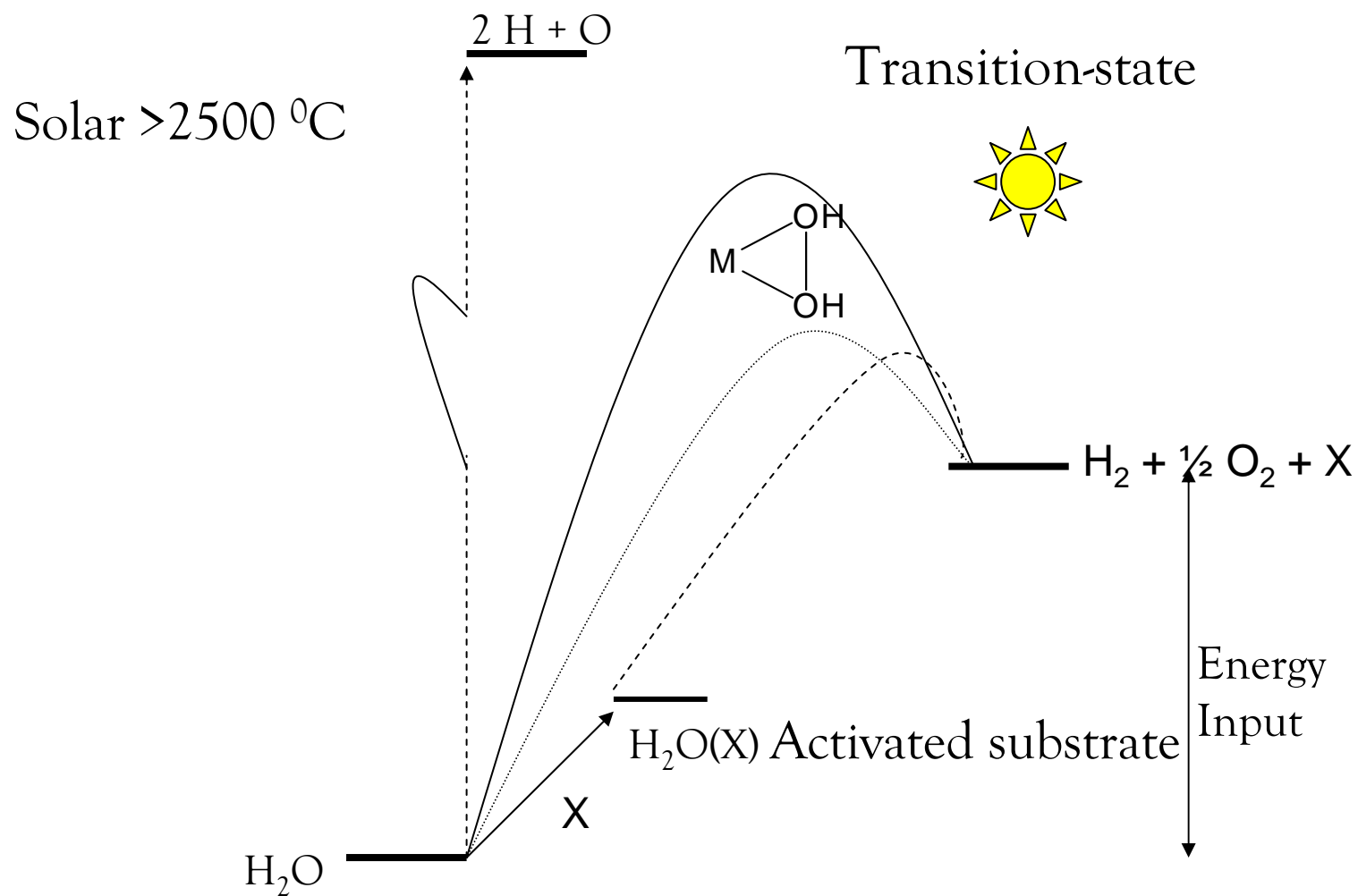
At steady-state, the Earth radiates as much energy as it absorbs, but the radiated photons have greater degrees of freedom.

# Proteins are '*Polanyi Machines*'

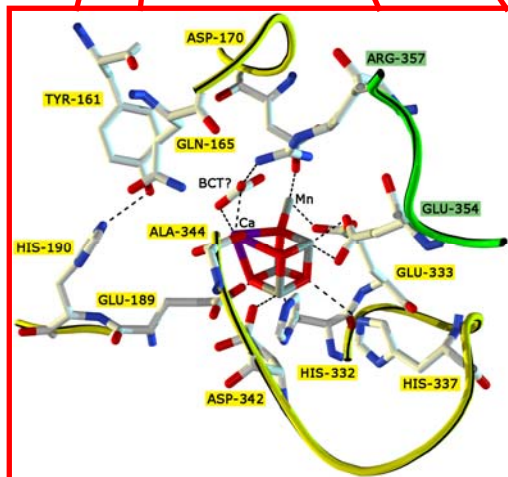
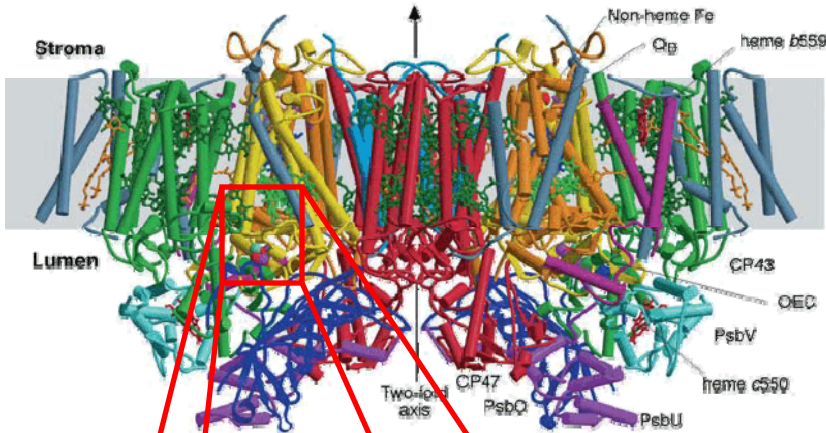
Living processes can be analyzed in terms of boundaries between distinctly different states of order. The elements of these 'surfaces' need not be connected.

The Sun-Earth 'boundary' is the set of all membranes containing photosynthetic proteins. On one side, free energy is in the form of photons, on the other it is contained in the chemical bonds of ATP.

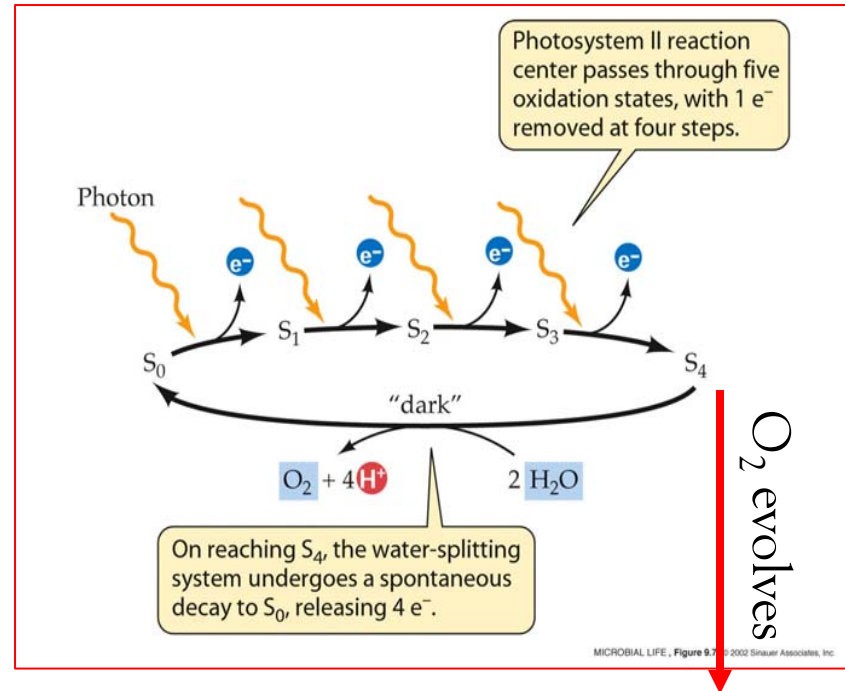
# Chemical Pathways for Catalyzing Water Splitting



# Oxygenic Photosynthesis

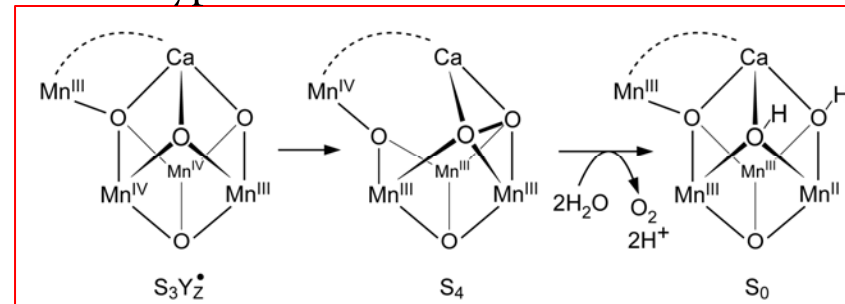


Ferreira *et al.* (2004) Science



MICROBIAL LIFE, Figure 8.7 © 2002 Sinauer Associates, Inc.

Hypothesized mechanism:



PS-II - the ultimate Polanyi Machine

# Biomimetic water-oxidizing complex

QuickTime™ and a  
YUV420 codec decompressor  
are needed to see this picture.

Entropy or Enthalpy?

Courtesy of Prof. Charles Dismukes, Princeton University

# Max Perutz on ‘What Is Life?’

“I wonder why Schrödinger did not adhere to Delbrück’s much better formulation of ‘a polymeric entity that arises by repetition of identical atomic structures’. One could argue over the distinction between aperiodic and identical, but Delbrück could not have meant structures that are completely identical, since these could contain no information.”

“Physics and the Riddle of Life”, *Nature* (326), 1987

# Protein cores are *aperiodic crystals*

Protein folding is driven by the entropy change of water molecules (Kauzmann, 1959).

QuickTime™ and a TIFF (Uncompressed) decompressor are needed to see this picture.

$$\Delta S_{\text{protein}} = \Delta S_{\text{chain}} + \Delta S_{\text{water}} \geq 0$$

ras p21

The hydrophobic cores of proteins are *close-packed*.  
(Richards, 1973).

# Max Perutz on ‘What is Life?’

“Chemists could also have told him that there is no problem in explaining stability of polymers that living matter is made of, because bond energies range from 3 eV upward, corresponding to a half-life of  $10^{30}$  years at room temperature”

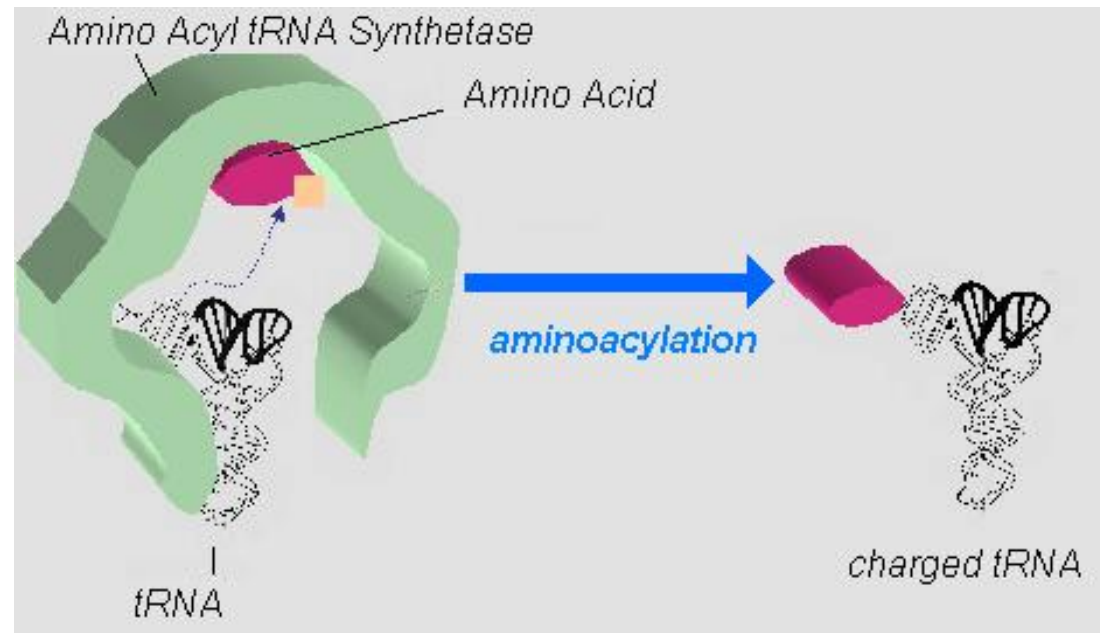
“The difficulty resides in explaining how their aperiodic patterns are accurately reproduced in each generation. There is no mention of this central problem in Schrödinger’s book”

“Physics and the Riddle of Life”, Nature (326), 1987

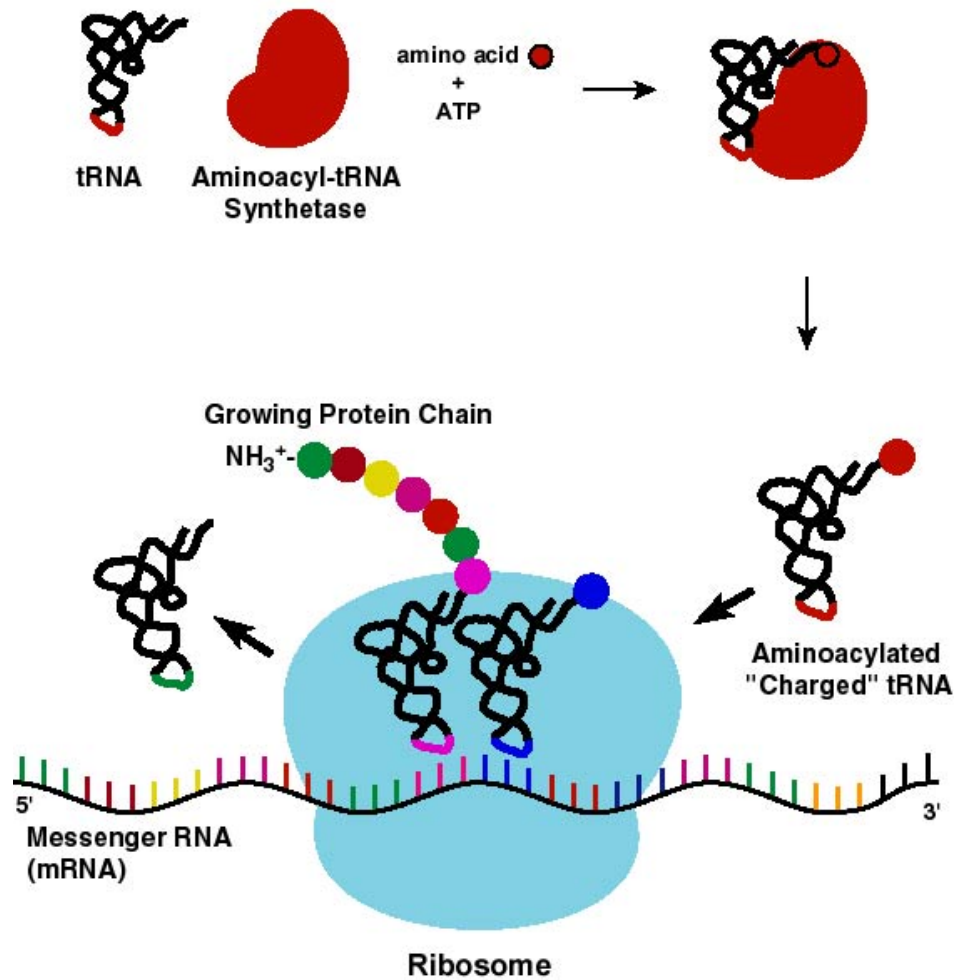


# amino-acyl t-RNA synthetases are Polanyi Machines

Protein synthesis can be conceptualized as a ‘disordered’ pool of the 20 different amino acids separated by a boundary having ‘ordered’ linear sequences on the other side. It takes Gibbs free energy to ‘sort’ and assemble the amino acids into polypeptide chains.



# Translation of the Genetic Code



# Thermodynamics of Sorting

Protein synthesis is a disorder-to-order process. Aminoacyl t-RNA synthetases select amino acids from a random pool.

$$v_A / v_B = [A]/[B] e^{-\Delta G_b/RT}$$

$\Delta G_b$  is the difference in binding energy of the side-chains,  
 $v_A$  is the rate of charging t-RNA.

# Protein Folding: The Second Code

The information contained within the one-dimensional amino acid sequence of a protein is sufficient to dictate its three-dimensional structure.

$$H_n (p_1, p_2 \dots p_n) = \sum p_i \log p_i$$

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TIFF (Uncompressed) decompressor  
are needed to see this picture.

QuickTime™ and a  
TIFF (Uncompressed) decompressor  
are needed to see this picture.

“The Shannon entropy”

Schrödinger could not have anticipated that polymers could spontaneously undergo a disorder to order process.

Strait & Dewey, ‘The Shannon Information Entropy of Protein Sequences’, Biophysical J. 71:148-155 (1996)

# TMV Self-Assembly: Disk to Helix

QuickTime™ and a  
TIFF (Uncompressed) decompressor  
are needed to see this picture.

The design of the whole is contained in the part.

D.L.D.Caspar

# Stuart Kauffman: “The Adjacent Possible”

“In his famous book, *What is Life?*, Schrödinger asks ‘What is the source of the order in biology?’ He arrives at the idea ... (of) a microcode carried in some sort of aperiodic crystal - which turned out to be DNA and RNA - so he is brilliantly right. But if you ask if he got the essence of what makes something alive, it’s clear he didn’t.”

Kauffman concludes that to be ‘living’ an organism not only replicates, but must do *work* on its surroundings to explore new niches and create for itself new *constraining structures* (e.g. membranes).

QuickTime™ and a  
TIFF (Uncompressed) decompressor  
are needed to see this picture.

# How do Polanyi machines perform reversible work?

$$\Delta G_{\text{life}} = \text{reversible work}_{\text{life}}$$

Protein machines doing work must control the (slow?) release of Gibbs free energy from ATP for maximum thermodynamic efficiency. Brownian motion must be kept to a minimum.

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TIFF (Uncompressed) decompressor  
are needed to see this picture.

# A.V. Hill: Energetics of Muscle Contraction

The astonishing thing about muscle is that the external load is transmitted directly to the energy producing molecules. It is akin to an electric motor where increasing the load results in more current in the coils (The Fenn Effect).

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TIFF (Uncompressed) decompressor  
are needed to see this picture.

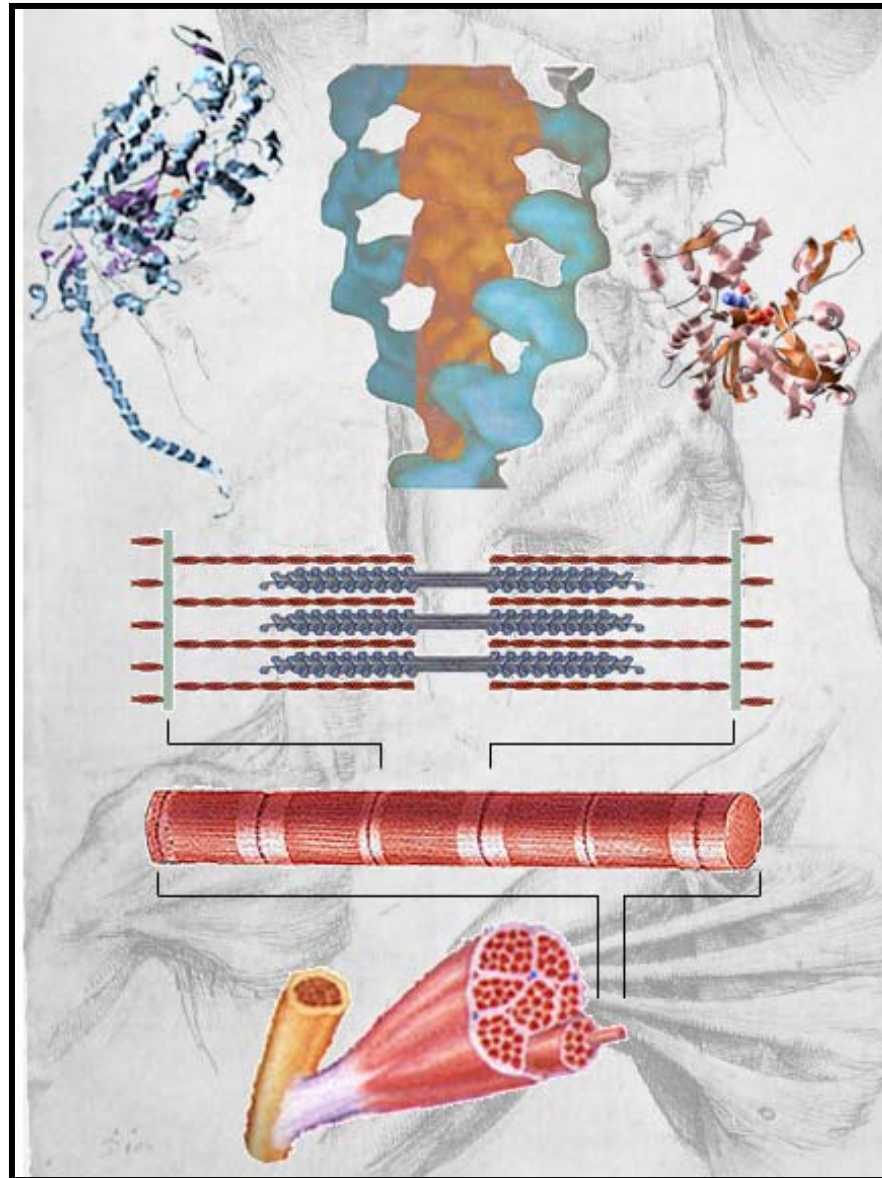
$$\text{Heat} + \text{work} = K(P_o - P)$$

1886-1977

Proc. Roy. Soc. B126, 136-195 (1938)

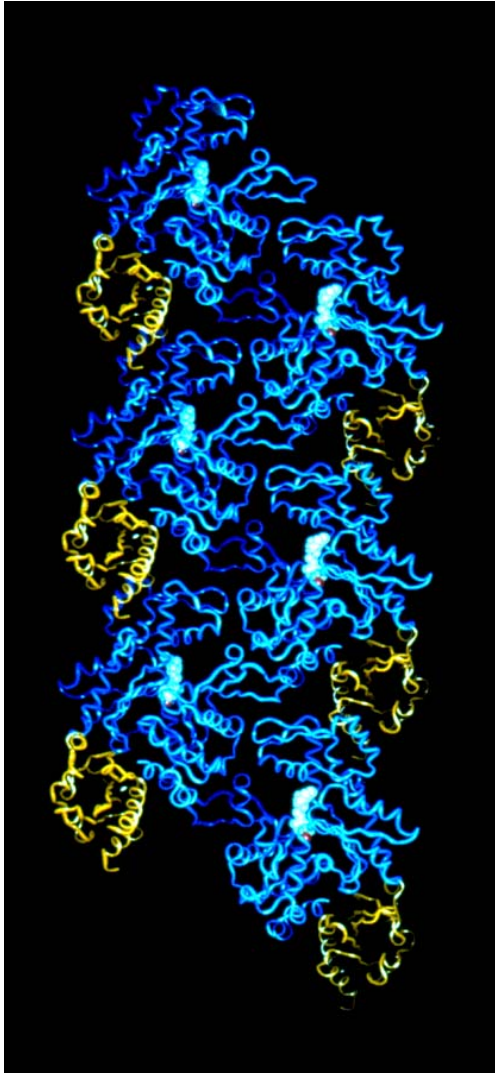


# 'Structure' as Hierarchical Ordering

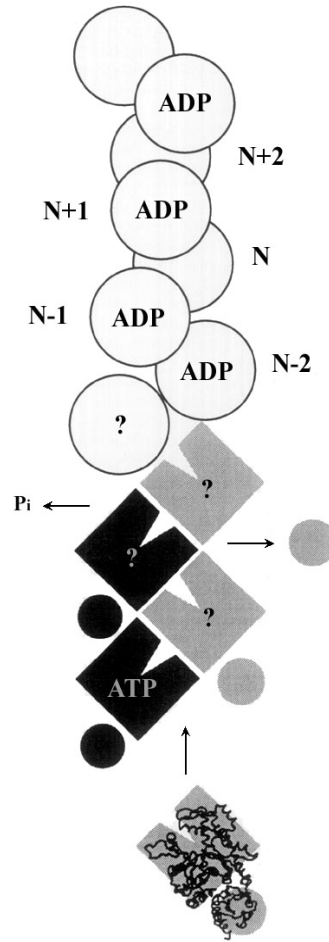


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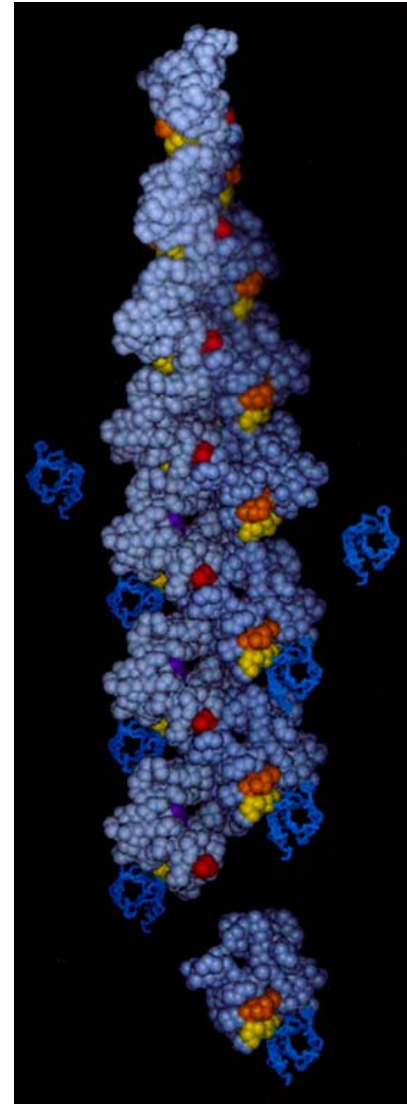
C.E. Schutt & U. Lindberg,  
“The New Architectonics: An  
Invitation to Structural Biology”  
*The Anatomical Record*, 2000



*Pointed End*

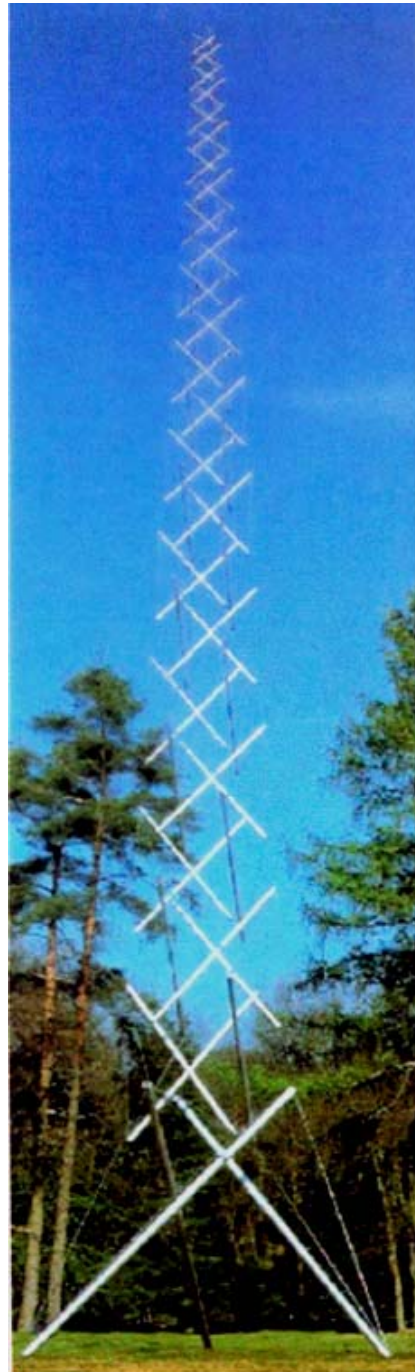


*Barbed End*



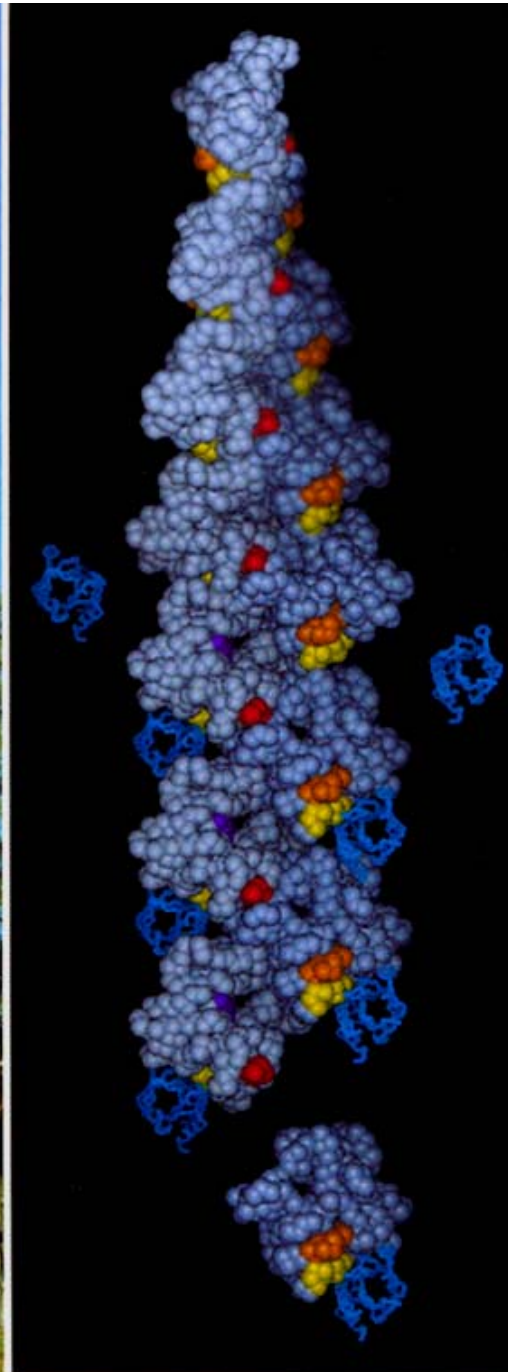
# Tensegrity Sculpture

Snelson



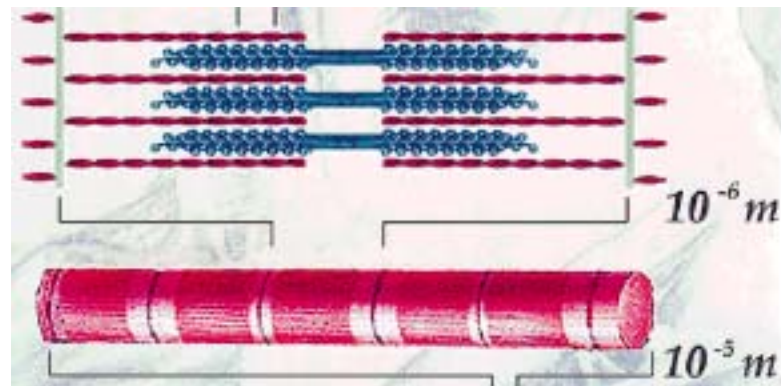
# Actin Filament

Schutt and Lindberg



# Functional Unit of Muscle Contraction

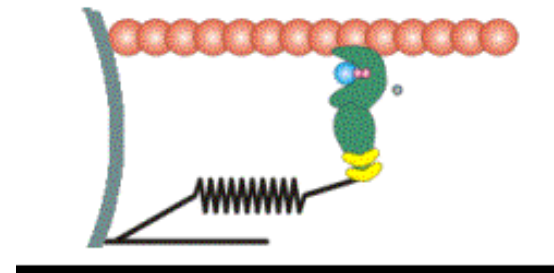
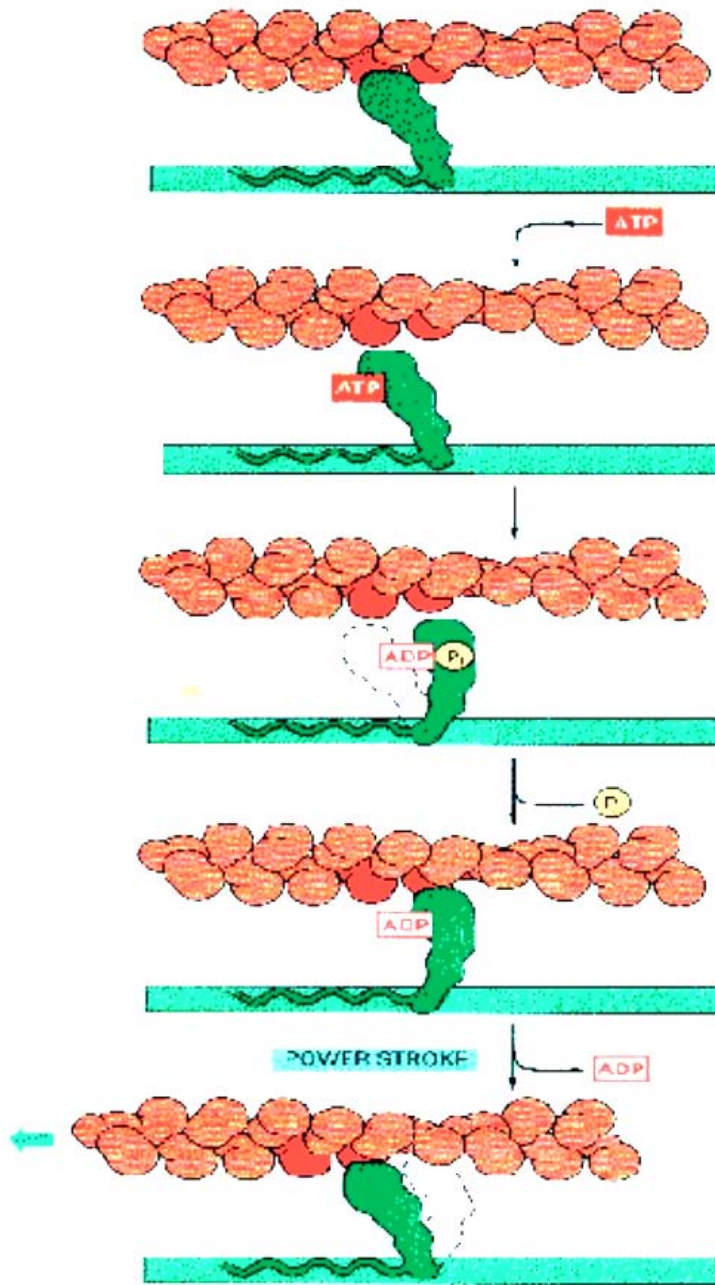
The sarcomere is the basic unit of muscle structure.  
Actin filaments (rosa) move relative to myosin filaments (azul).



Central question: what drives the relative motion?

Huxley & Hansen (1954), Huxley & Neidengerke (1954)

# Myosin Motor Model (passive actin filaments)



Huxley-Simmons, 1971

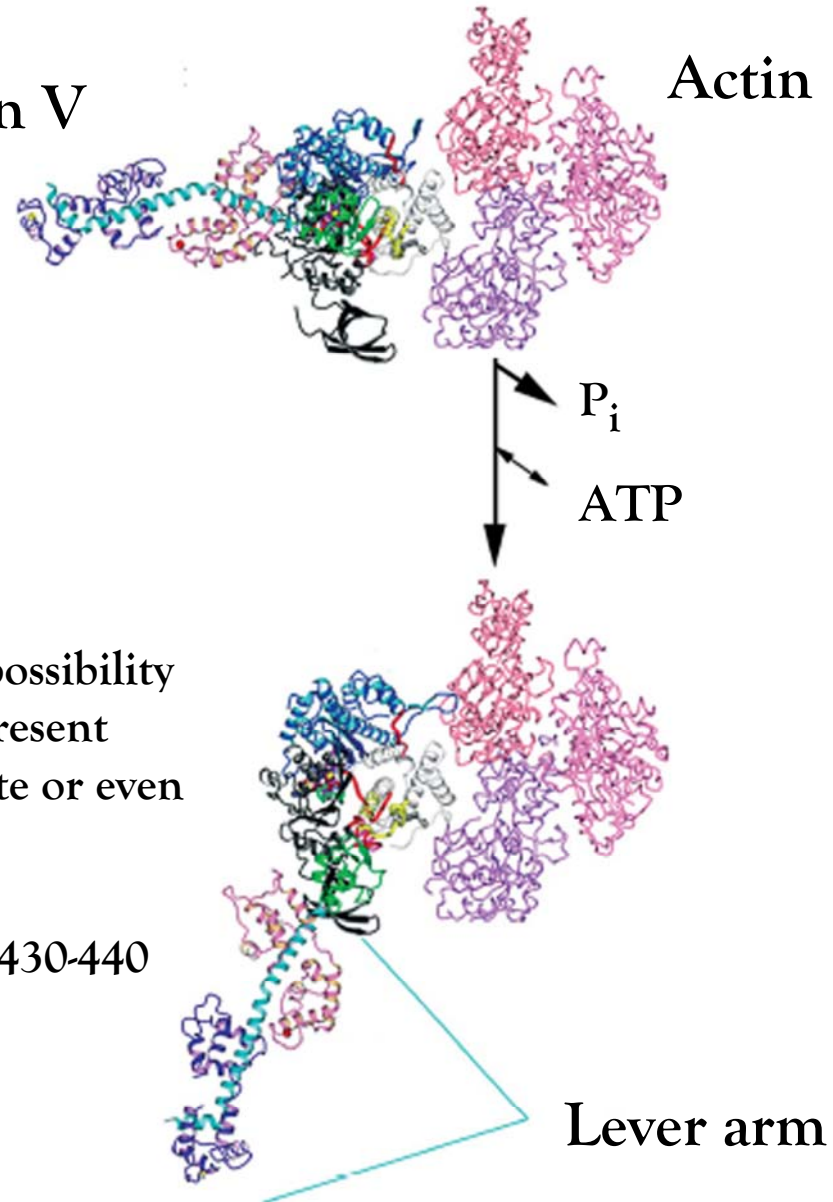
Myosin V

Actin

## The swinging cross-bridge theory

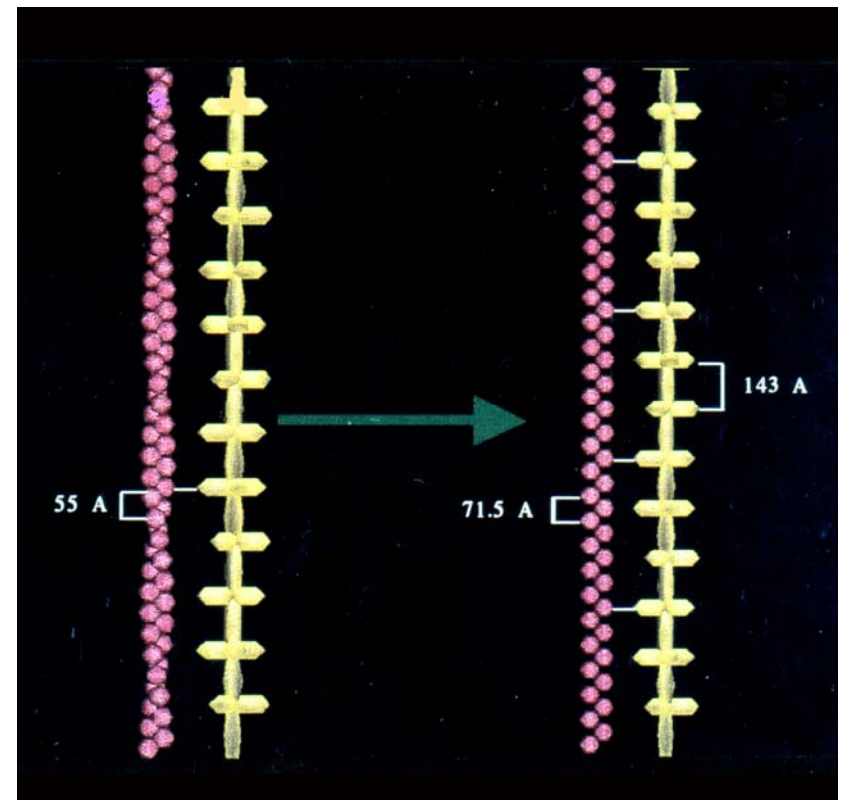
“Apart from such quantitative uncertainties, there is always a possibility indeed, a probability that our present concepts are seriously incomplete or even wrong.”

AF Huxley *Proc Roy Soc* 2004 430-440



# Commensurability At Work: The Third Architectonic Principle?

In our view, actin 'thin filaments' can interconvert between the classical helical state and a ribbon state (having the same longitudinal spacing as the myosin headgroups on 'thick filaments').



# A New Theory of Muscle Contraction

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TIFF (Uncompressed) decompressor  
are needed to see this picture.



# Principle of Actin Motor

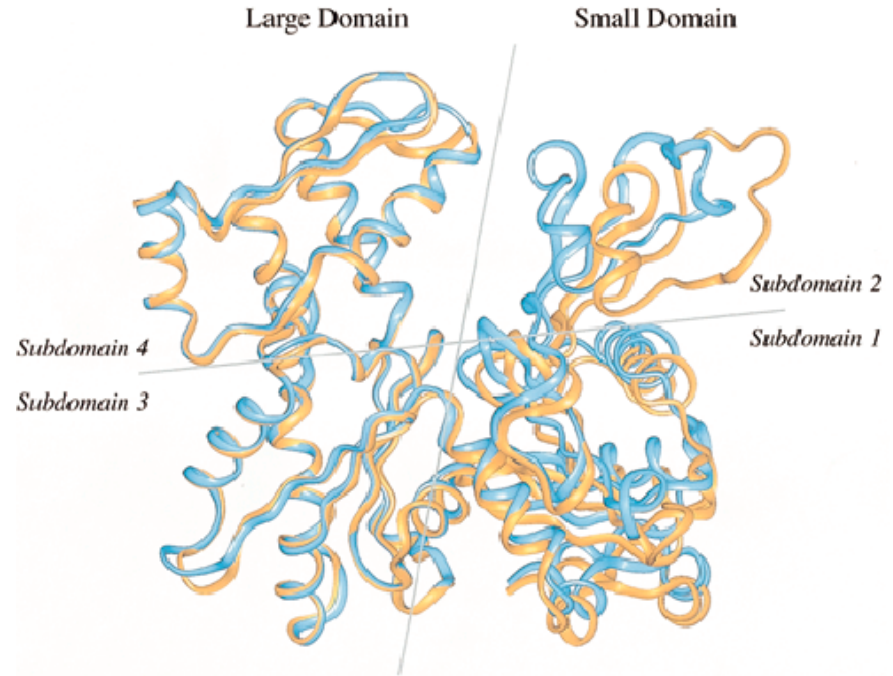
Conformational change in actin in the direction of motion accompanies ATP hydrolysis

$$F = - \frac{\varepsilon \cdot \Delta G}{\Delta x}$$

$\Delta G$  is the free energy of ATP hydrolysis.

$8.0 \times 10^{-20}$  J/ATP molecule

Force = 200 pN



Chik, Lindberg & Schutt, 1996  
Page, Lindberg & Schutt, 1998

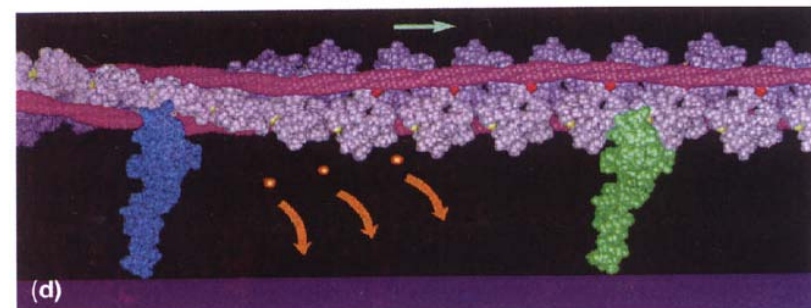
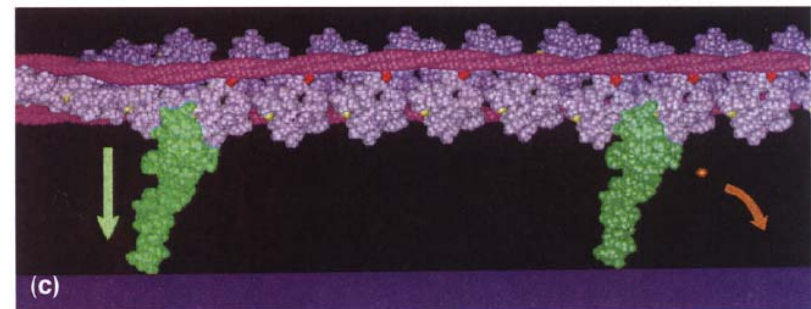
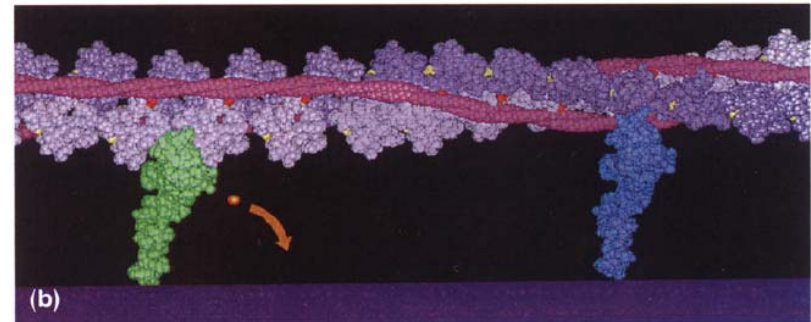
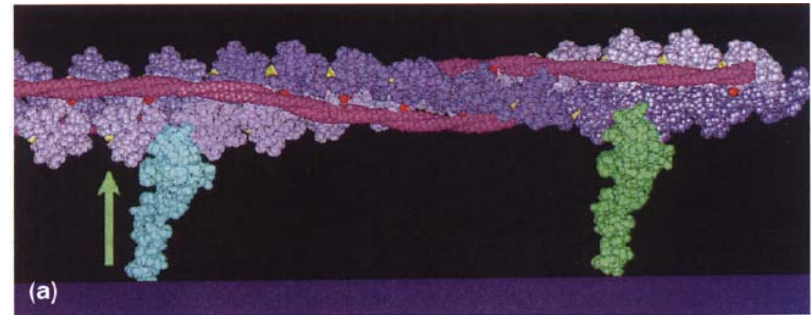
# Actin Motor Model

(a) Myosin induces a change in actin filaments.

(b) The change is propagated along actin filaments.

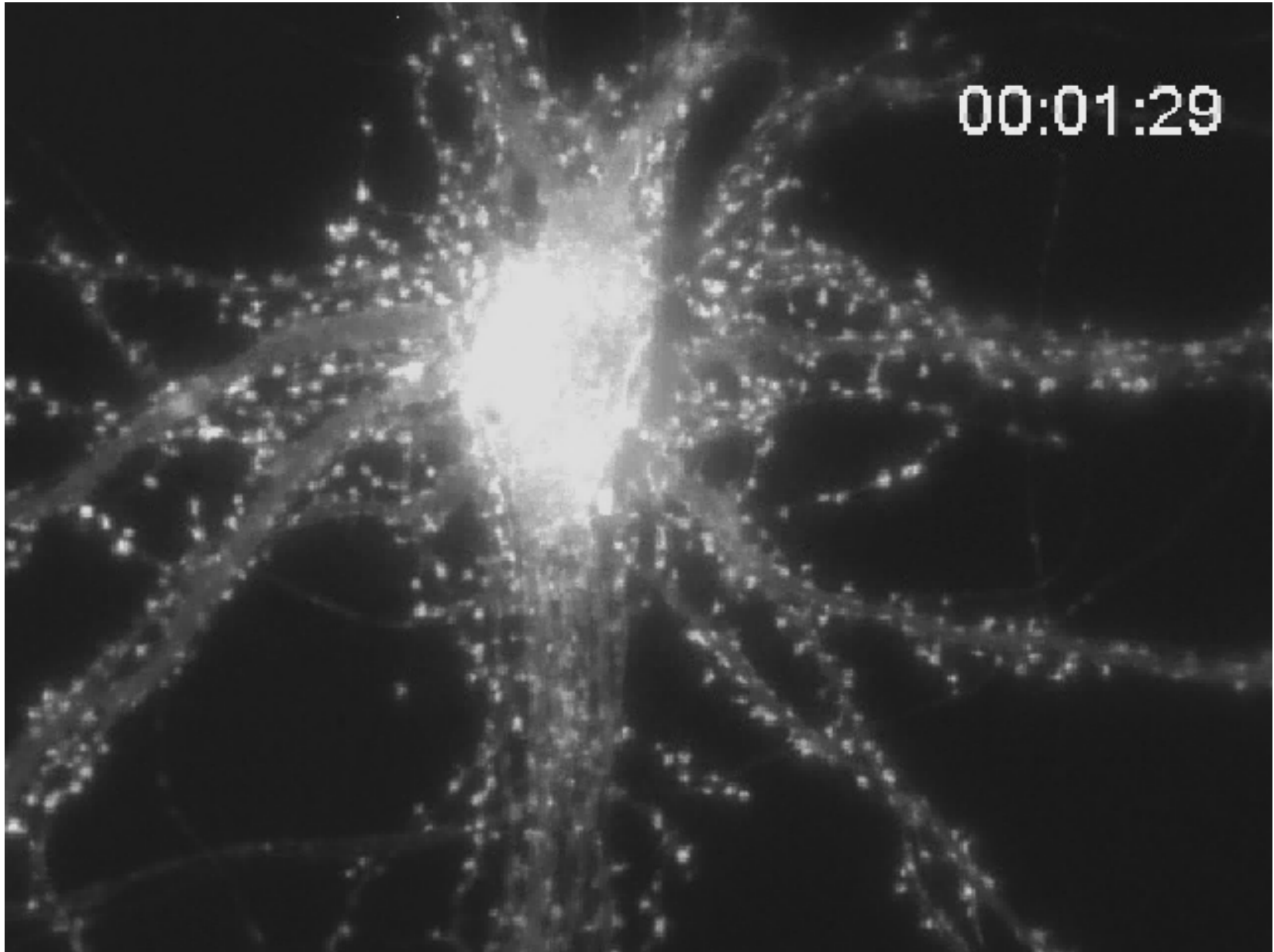
(c) ATP is hydrolyzed on actin.

(d) Force is generated as actin expels phosphate.



"Everything is movement; thought is a movement; life is based on movement; death is a movement to which the end escapes us. If God is eternal, you may be sure he is always in motion. God is perhaps movement itself. That is why movement, like him, is inexplicable - like him, profound, without limits, incomprehensible, intangible."

Honore de Balzac ("Peau de Chagrin")



"It is a landscape that offers itself up to contemplation like an endless plastic wonder whose beauty is as mysteriously static and changing as that of the stars."

Video: Andrew Matus

Mario Vargas Llosa ("Szyszło")

