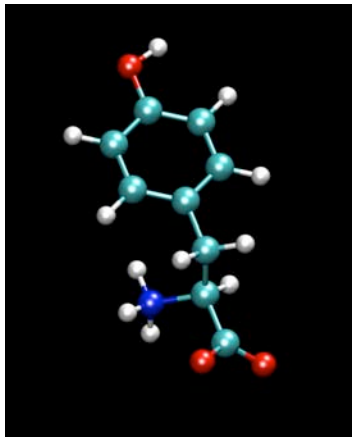
Lecture 1a

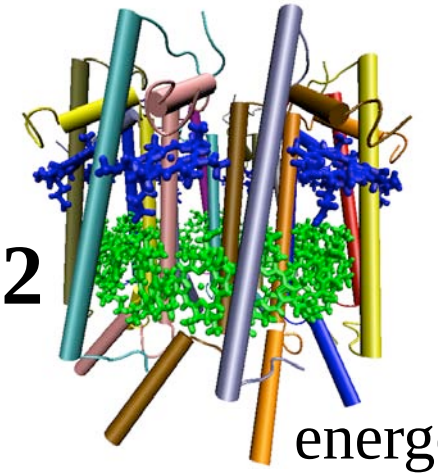
Introduction to Protein Structures - Molecular Graphics Tool



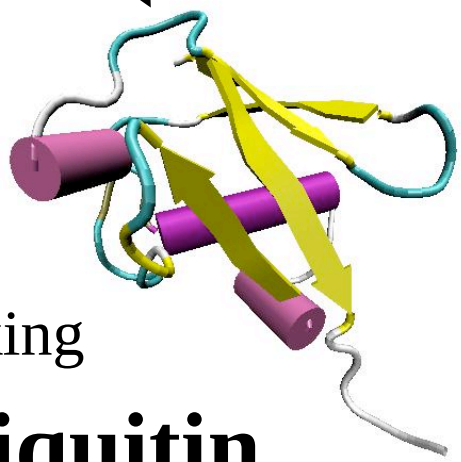
amino acid

tyrosine

LH2

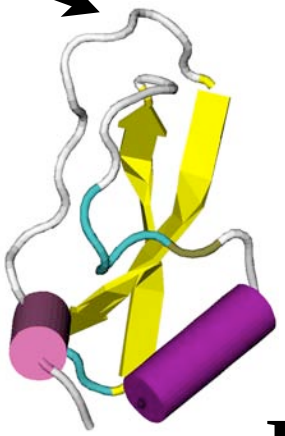


energetics



traficking

Ubiquitin

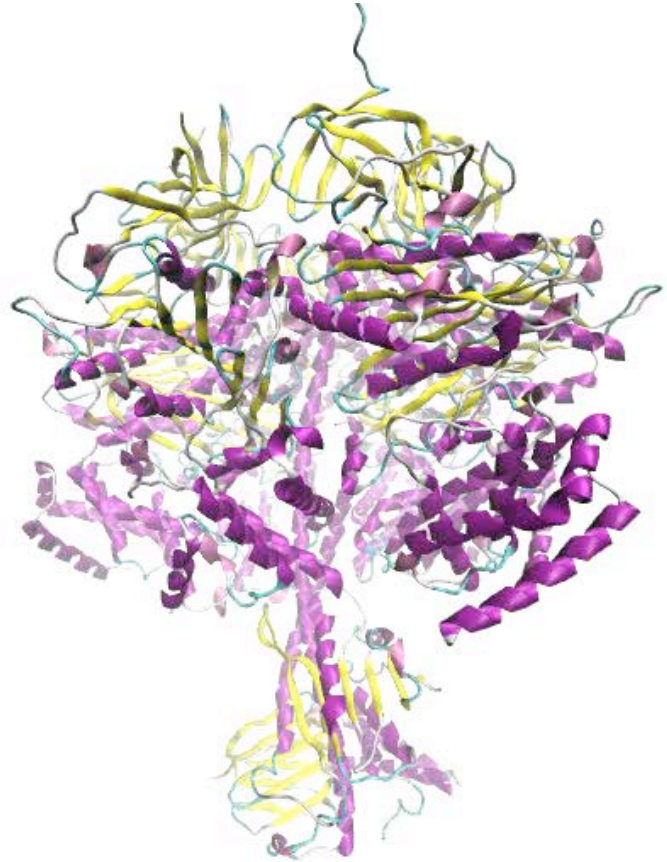


enzymatic control

BPTI

Highlights of the VMD Molecular Graphics Program

- > 120,000 registered users
- Platforms:
  - Unix / Linux
  - Windows
  - MacOS X
- Display of large biomolecules and simulation trajectories
- Sequence browsing and structure highlighting
- Multiple sequence - structure analysis
- User-extensible scripting interfaces for analysis and customization

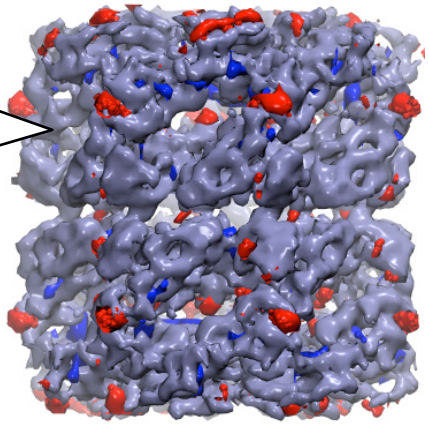


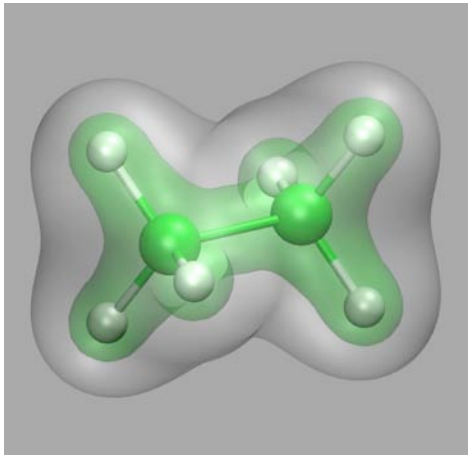
The program is used today more for preparation and analysis of modeling than for graphics

VMD – A Tool to Think

Volumetric Data:
Density maps,
Electron orbitals,
Electrostatic potential,
Time-averaged occupancy, …

23,000 Users

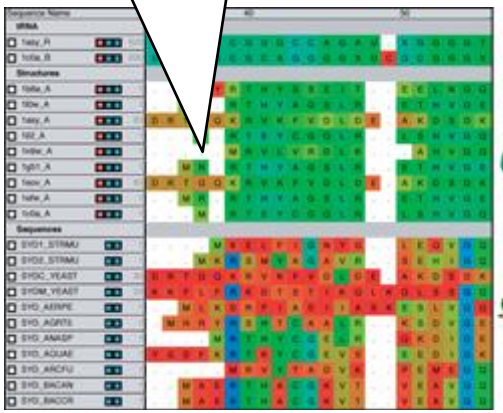


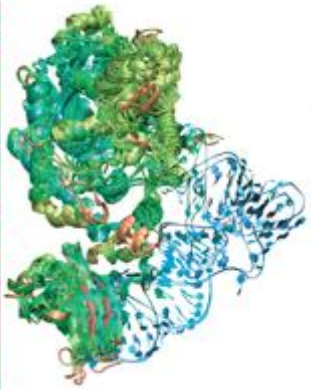


Sequence Data:
Multiple Alignments,
Phylogenetic Trees

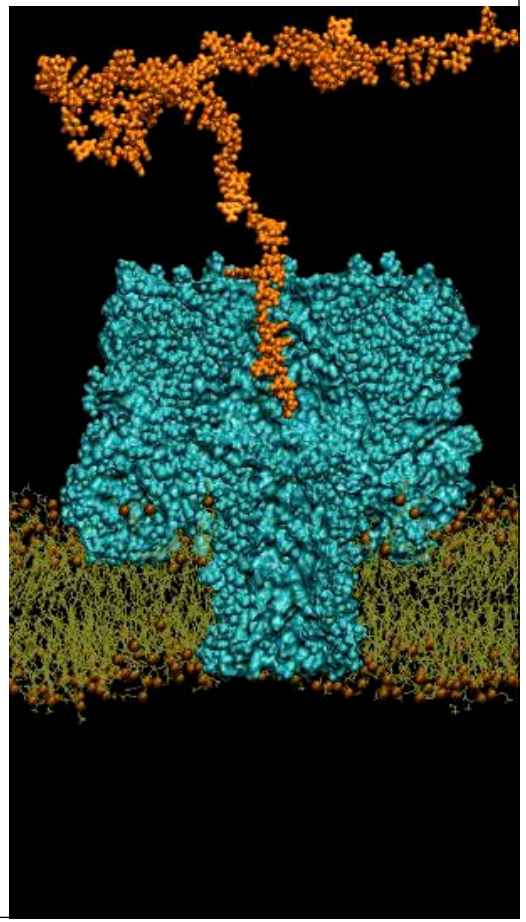
VMD

Annotations





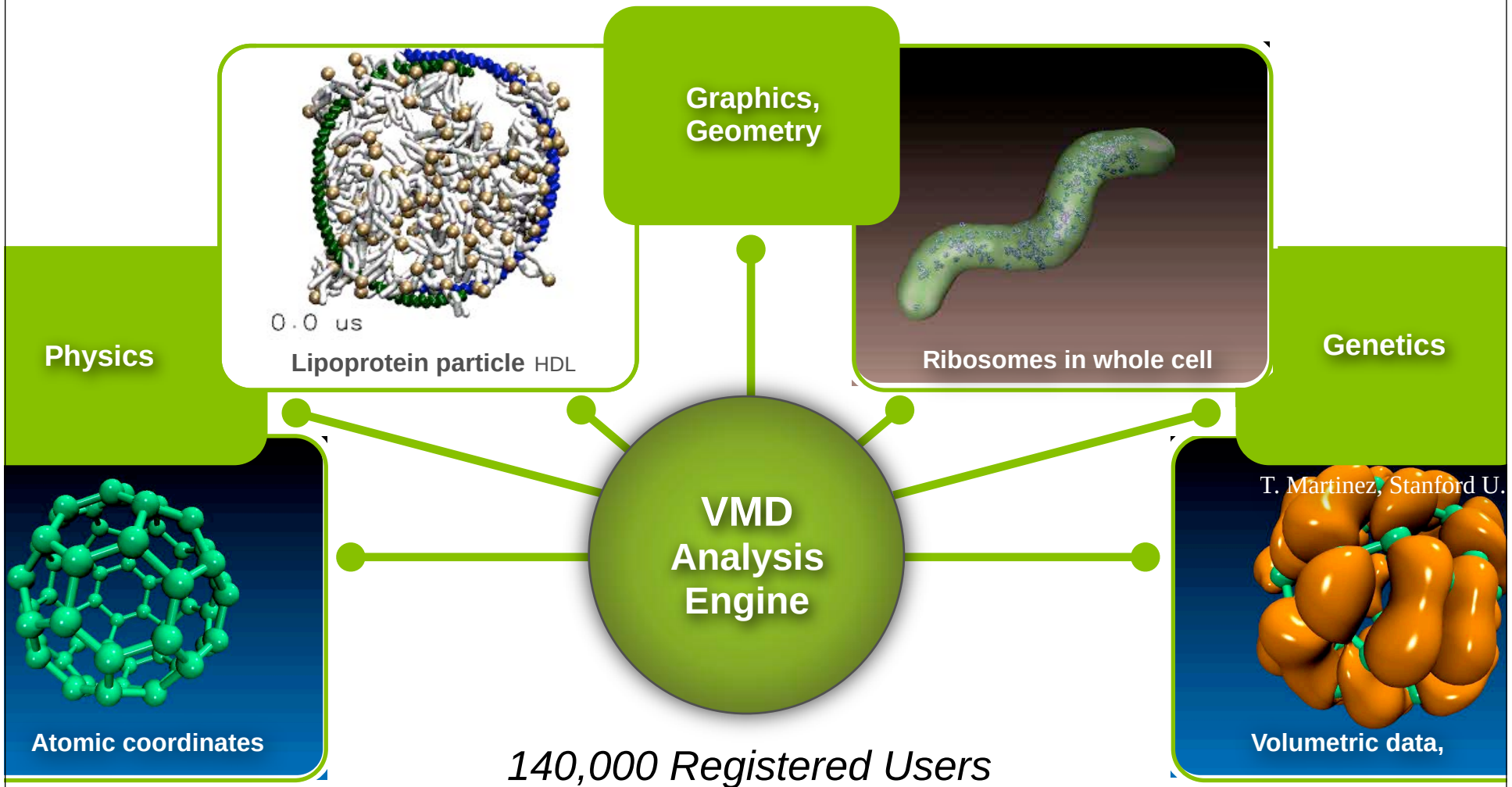
Atomic Data:
Coordinates,
Trajectories,
Energies,
Forces, …



National Center for Research Resources

VMD a “Tool to Think”

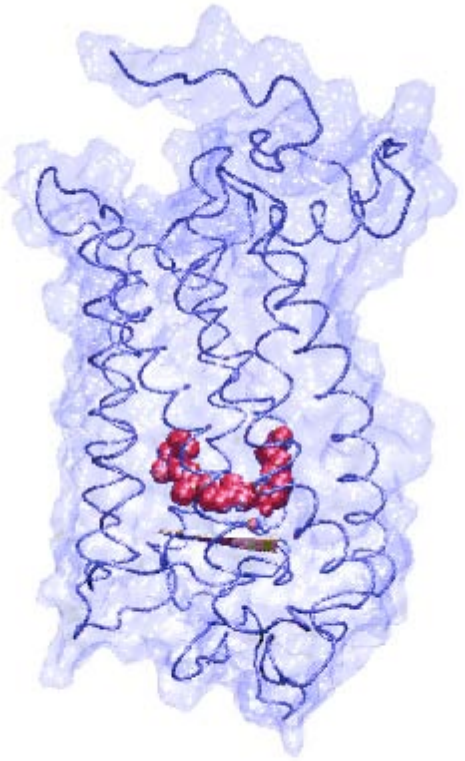
Carl Woese

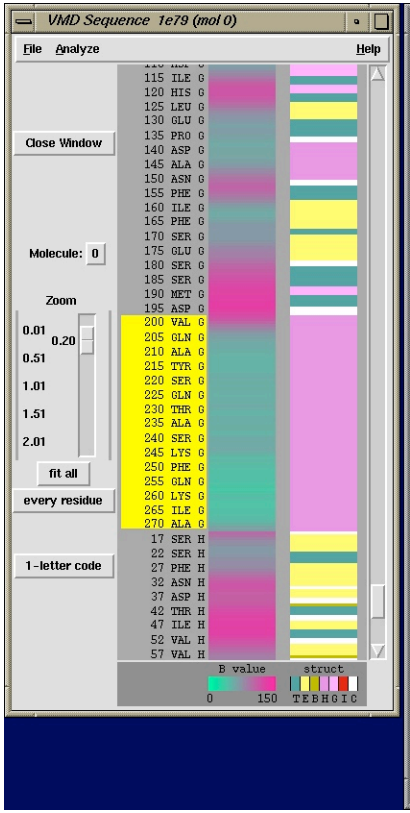


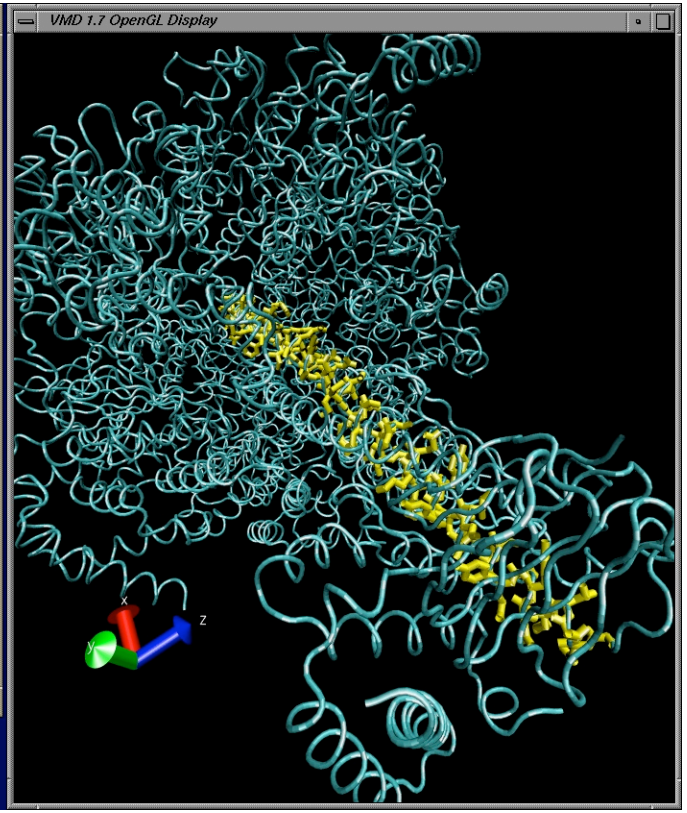
140,000 Registered Users

Molecular Graphics Perspective of Protein Structure and Function

see tutorial at http://www.ks.uiuc.edu/Training/Tutorials/



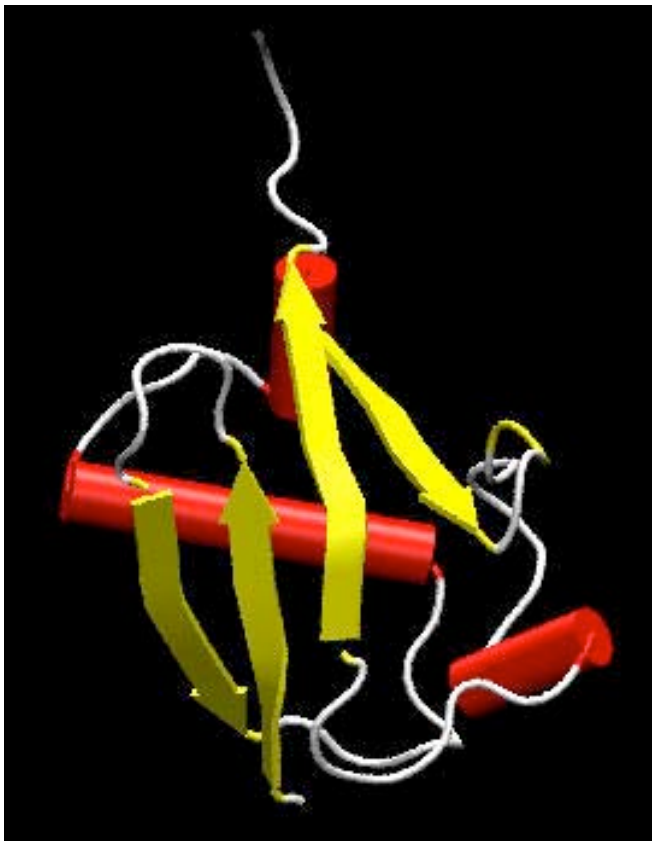




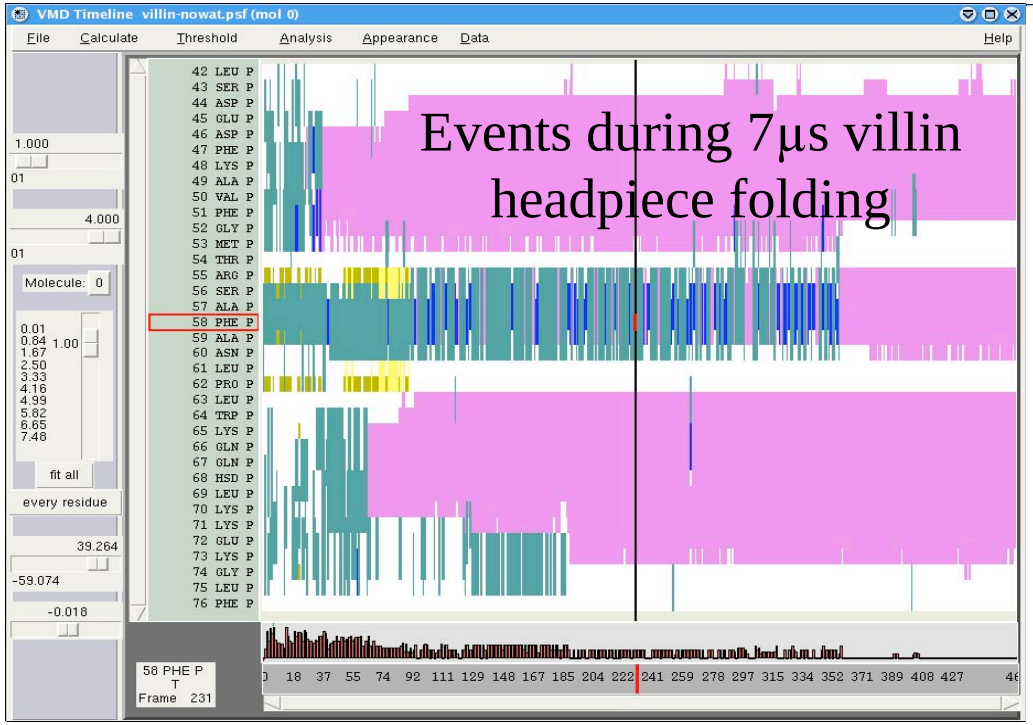
animation sequence structure

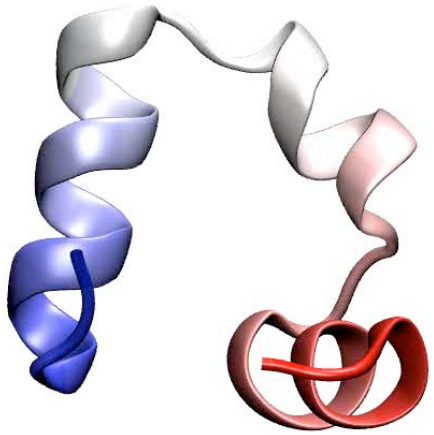
Ubiquitin

- 76 amino acids
- highly conserved
- covalently attaches to proteins and tags them for degradation
- other cell traficking



VMD New Timeline plug-in





Alpha helix Extended beta Isolated bridge 3-10 helix Beta turn None (coil)

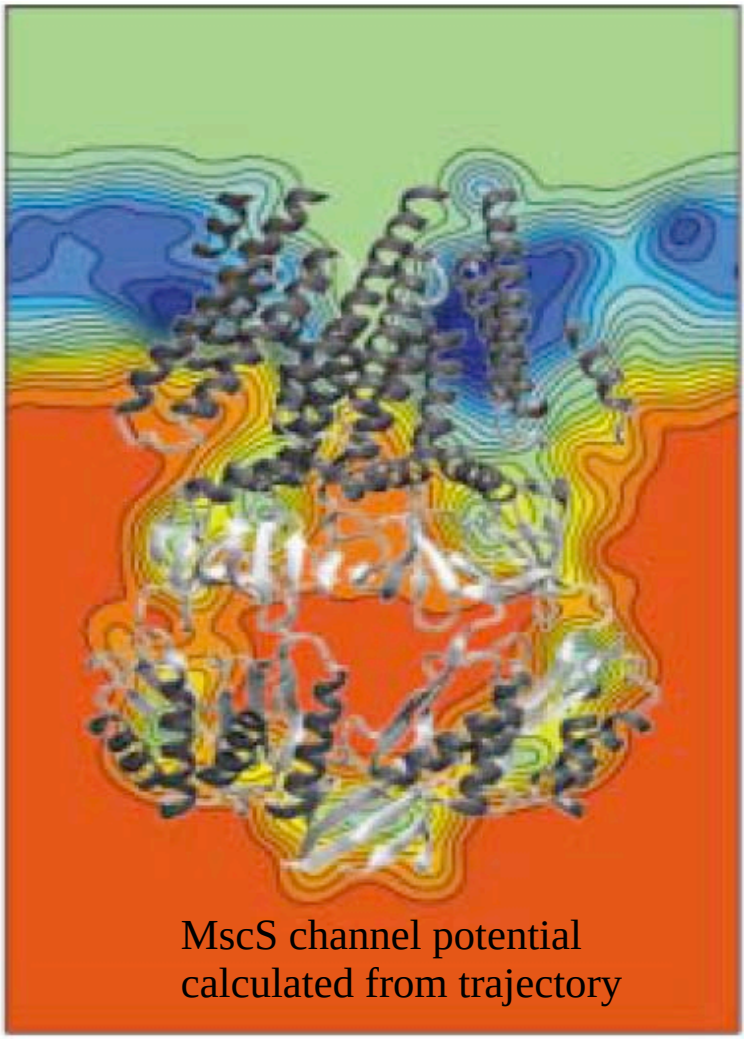
Per-residue secondary structure: villin headpiece folding from a fully denatured state.
7μs simulation; 654 atoms; over 1 million frames to examine

VMD **Timeline plug-in**: graphing and analysis tool to identify events in an MD trajectory
- a single picture shows changing properties across entire structure, entire trajectory.
- explore time vs. attribute (per-residue or per-selection) linked to molecular structure
- many analysis methods available; user-extendable

Electrostatic Potential Maps

New VMD features made possible through GPU computing

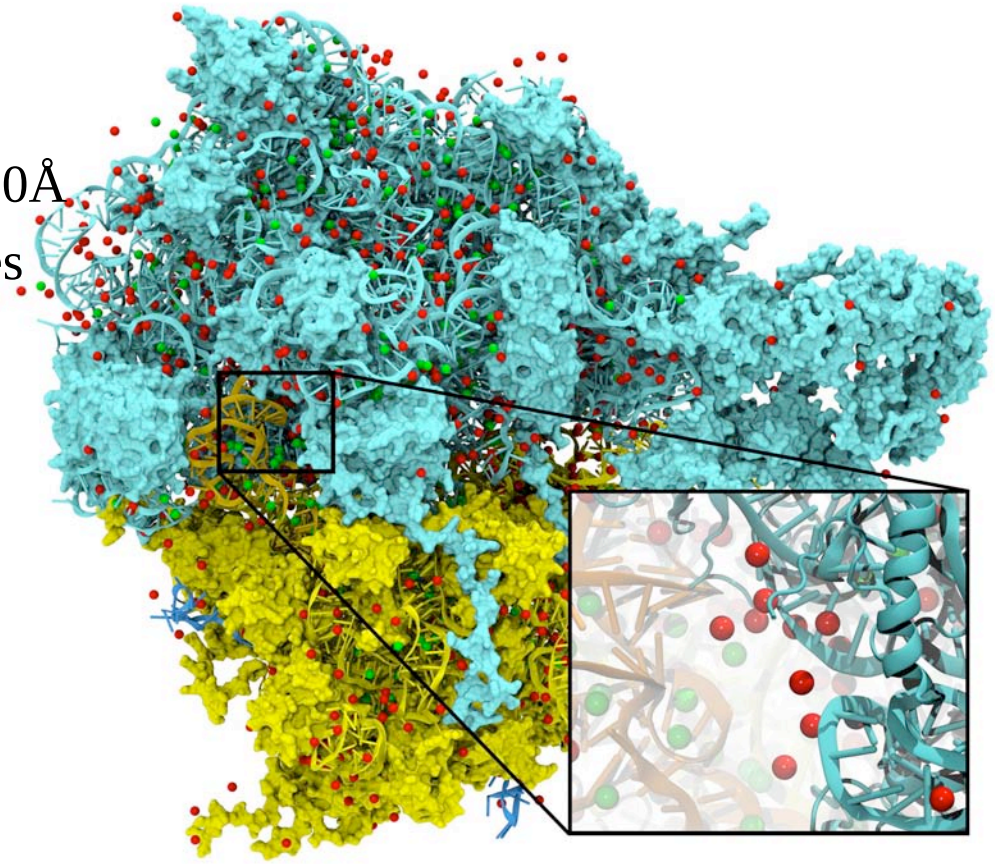
- Electrostatic potentials evaluated on 3-D lattice
- Applications include:
  - Ion placement for structure building
  - Time-averaged potentials for simulation
  - Visualization and analysis



MscS channel potential calculated from trajectory

Time-averaged Electrostatic Potential Calculation for the Ribosome with VMD

- Direct Coulomb summation ~580,000 atoms
  - Lattice spacing 1.0Å, padding 10Å
  - Time-average from 1,000 frames
- 3 GPUs: 49 hours
- 3 CPUs: 0.23 years (est.)

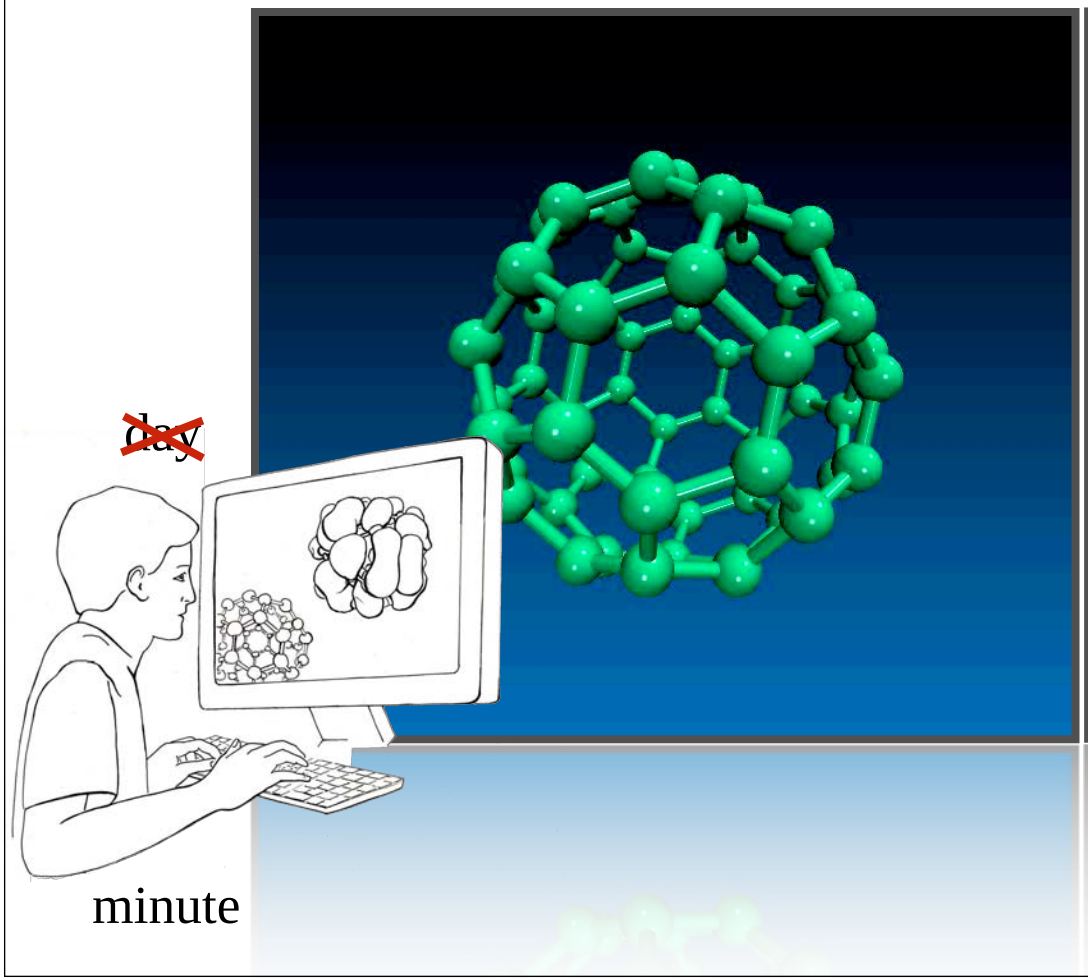


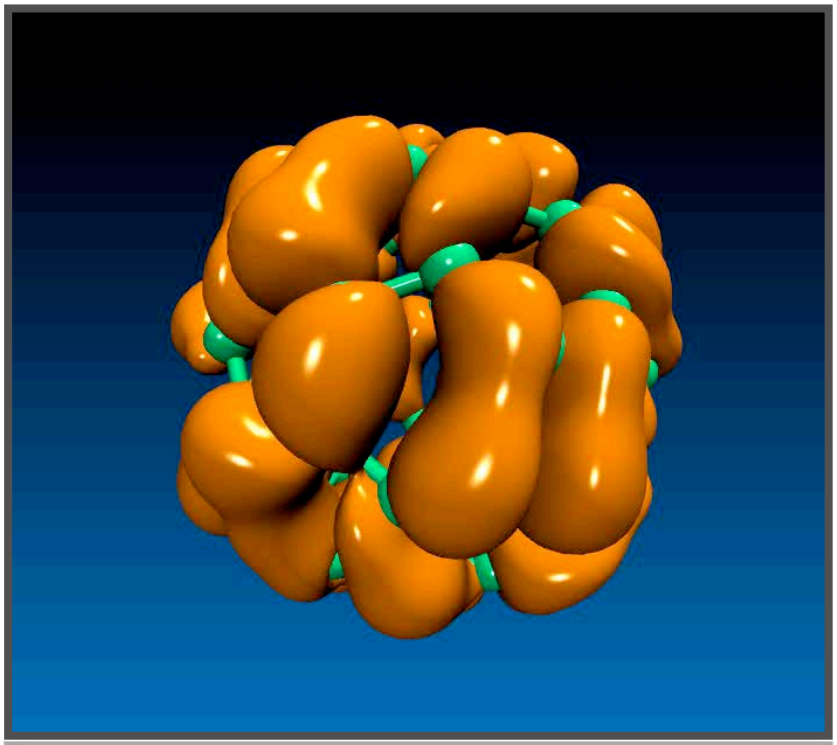
This was one of our early results, using the multi-GPU direct Coulomb summation algorithm, showing the benefit it gave at the time. Now that we have MSM (multilevel summation) we would get much faster performance since it is a linear-time algorithm, but we haven't yet re-run these tests using MSM.

Stone et al. (2007) *J Comp Chem* 28:2618-2640

Quantum Chemistry Visualization

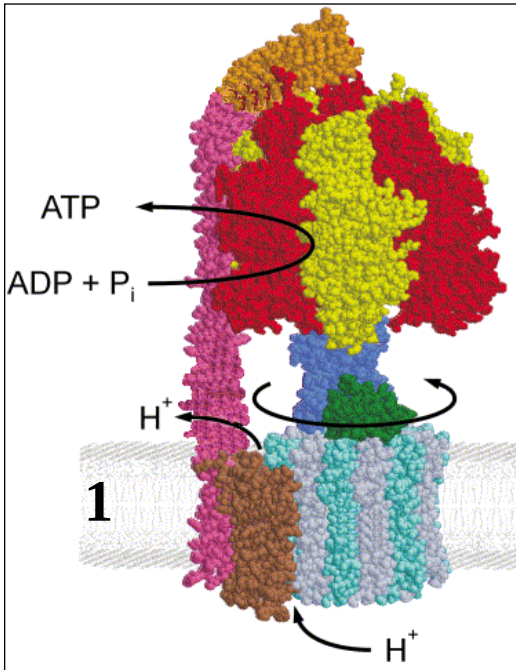
Rendering of electron “clouds” achieved on GPUs as quickly as you see this movie! CPUs: One working day!

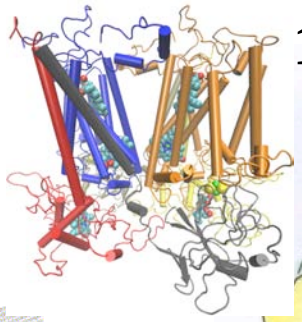




Simulation: Terachem Interactive Visualization: VMD
Courtesy T. Martinez, Stanford

The proteins that make up the chromatophore of photosynthetic bacteria

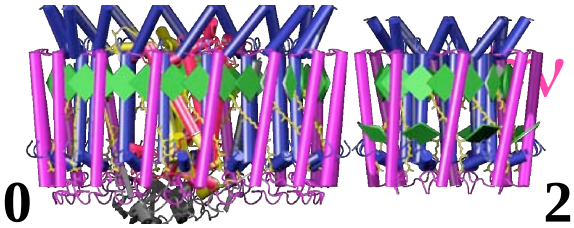




10

1

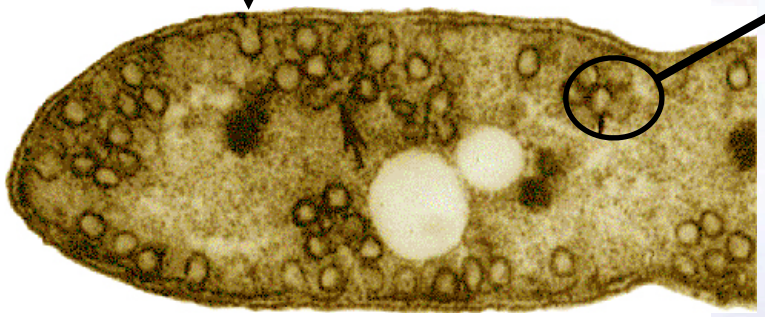
5



20

200

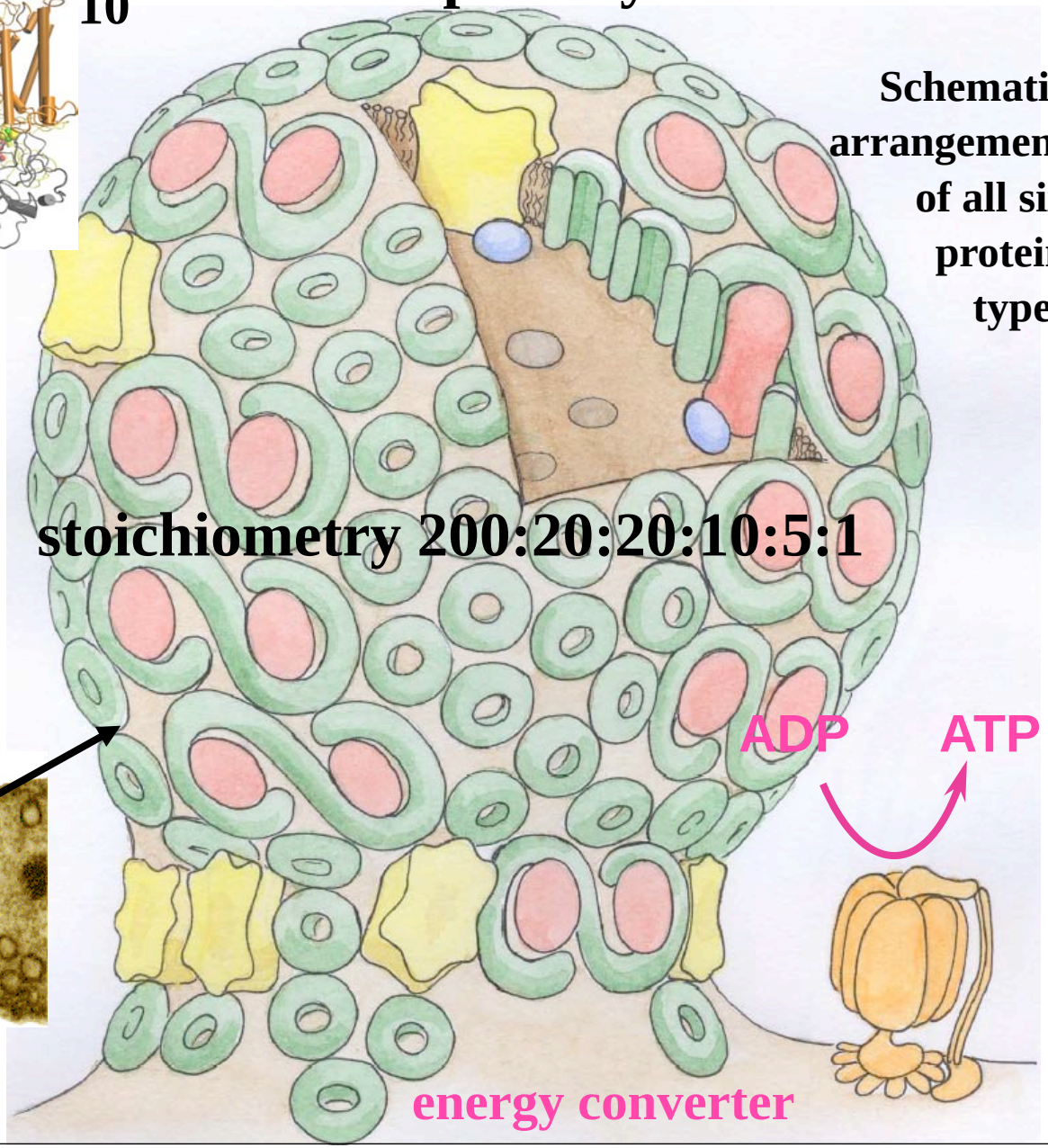
photosynthetic unit



purple bacterium cell

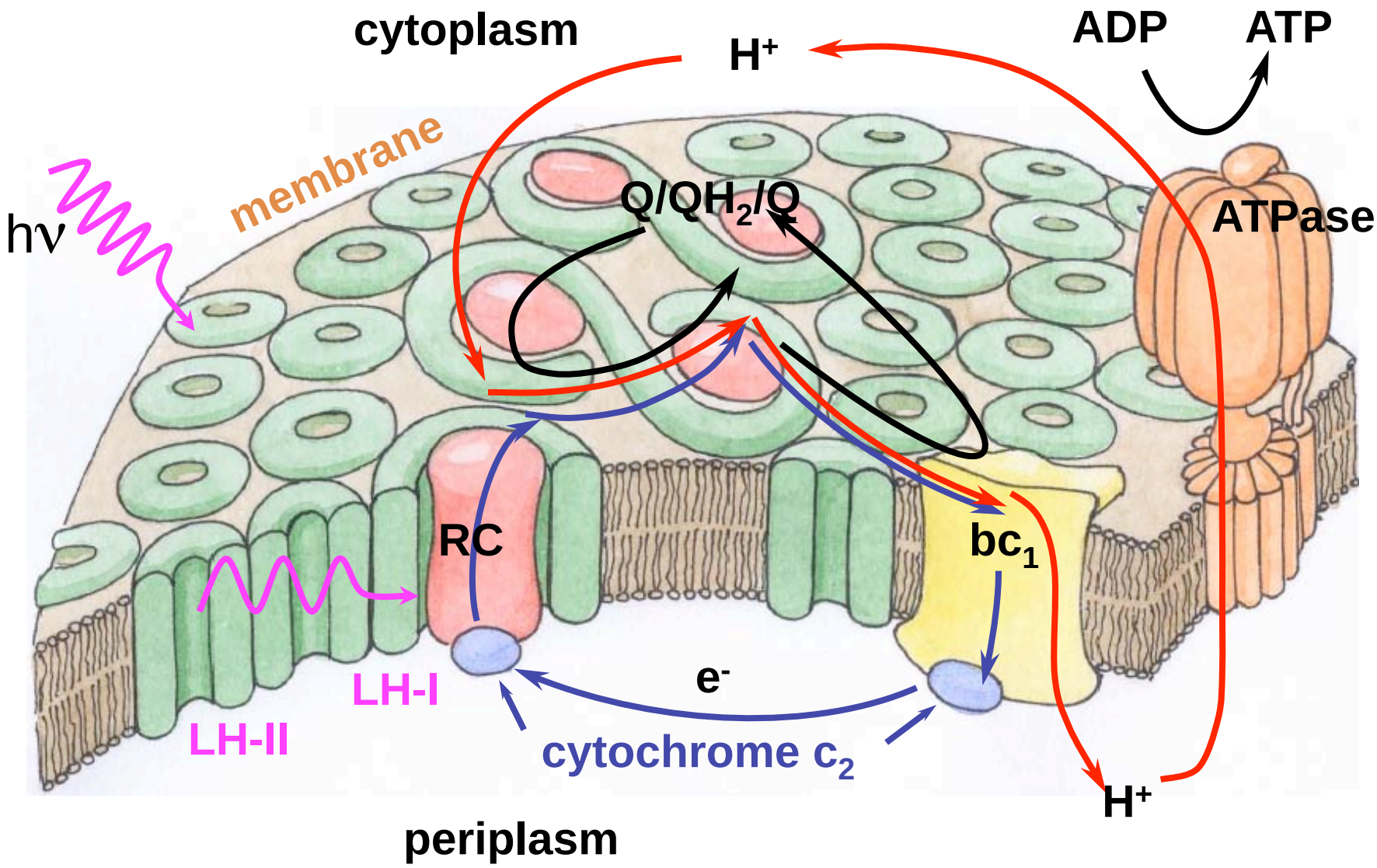
Schematic arrangement of all six protein types

stoichiometry 200:20:20:10:5:1

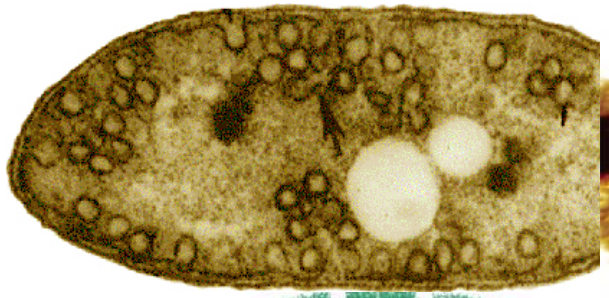


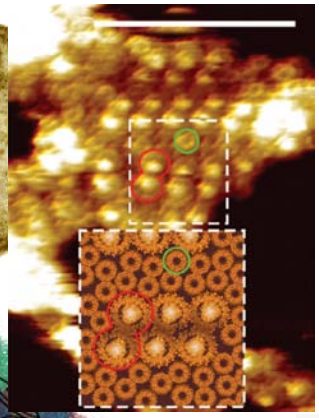
Chromatophore of Purple Bacteria

(section of the chromatophore membrane)

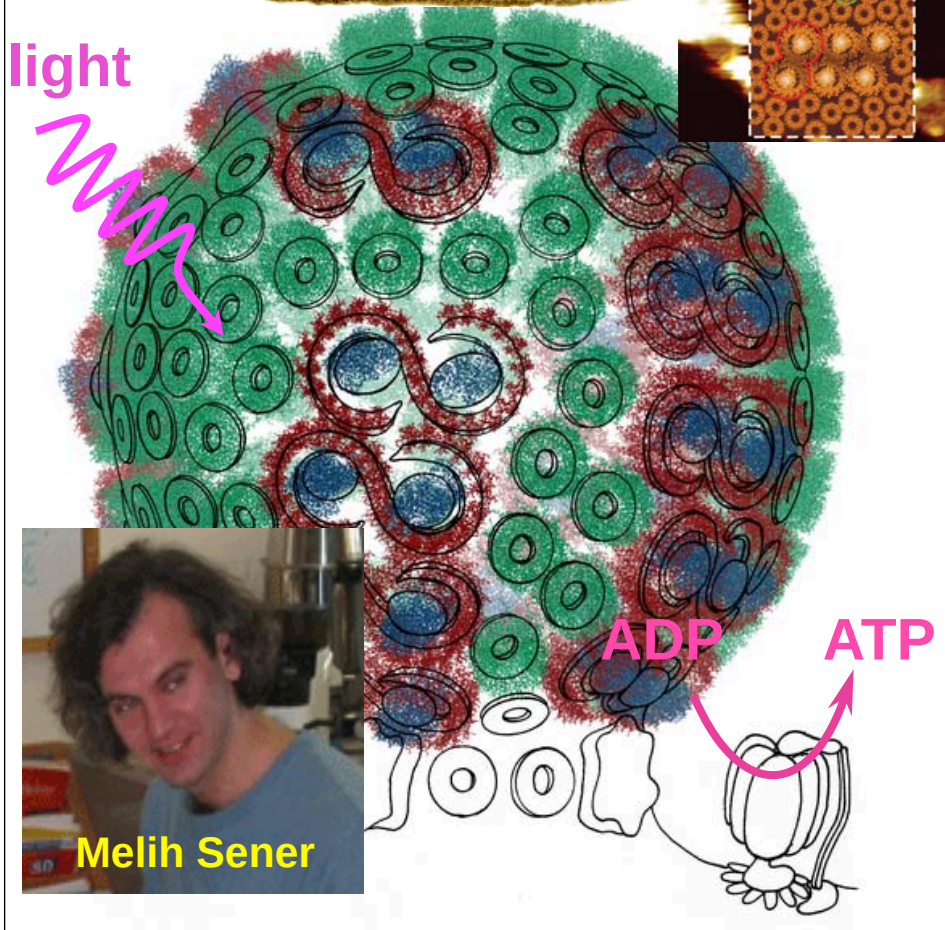


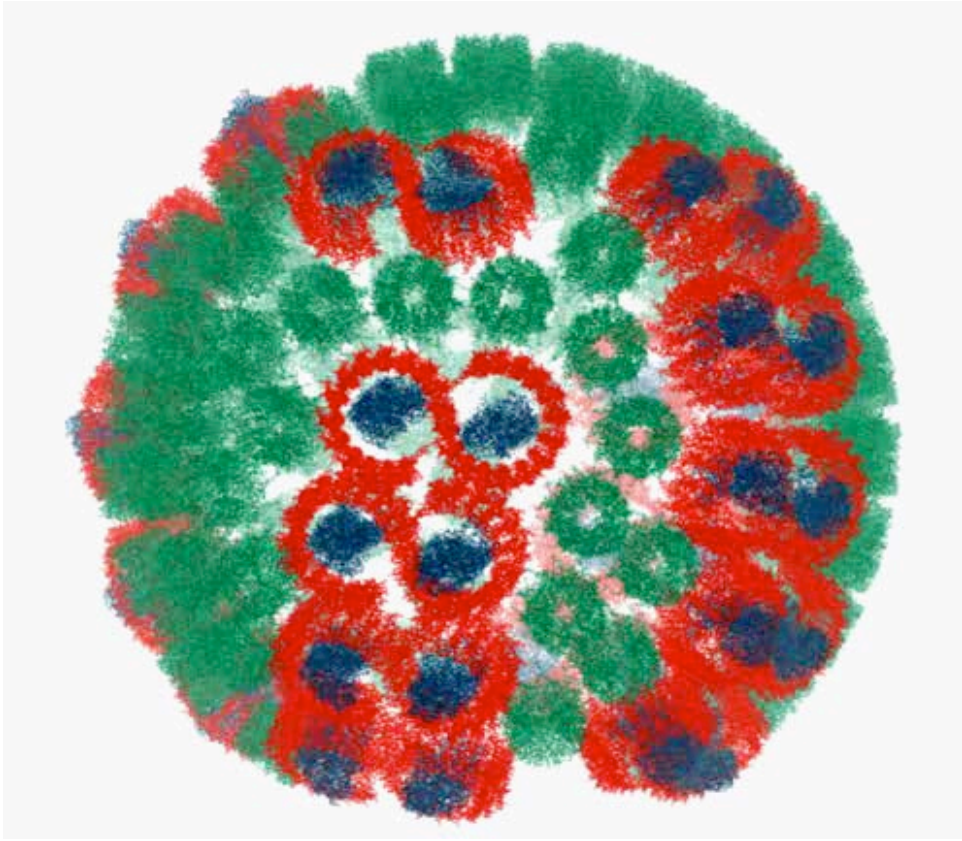
Knowing the Atomic Level Structure





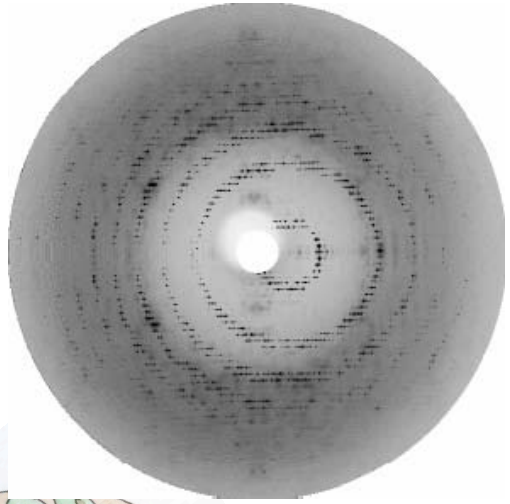
of the chromatophore, one can systematically describe its physical mechanism



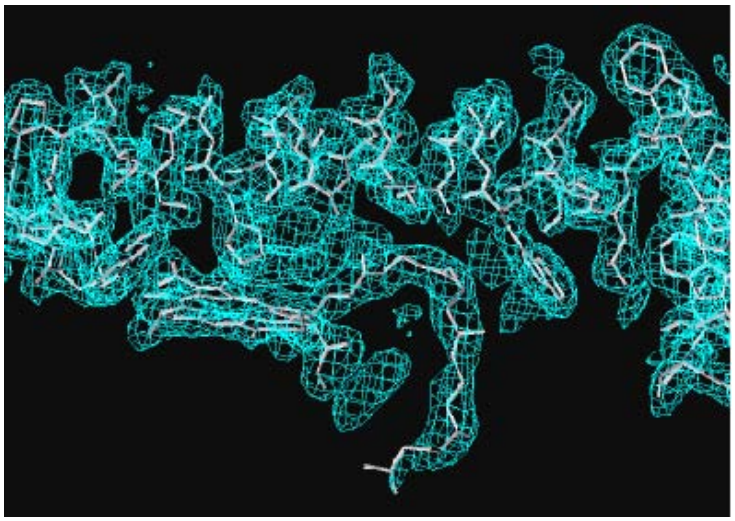


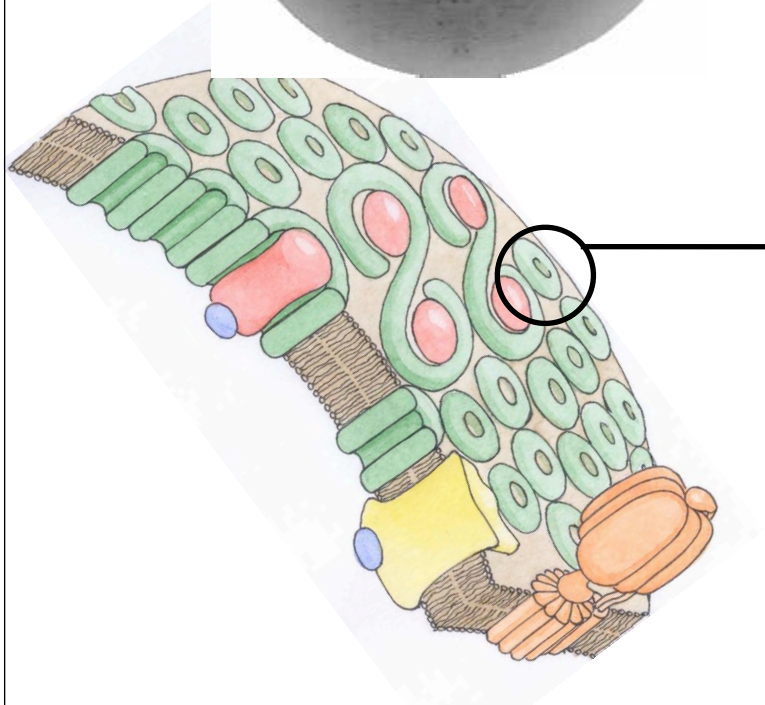
M. Sener, J. Olsen, N. Hunter, and K. Schulten. *PNAS*, **104:** 15723-15728, 2007

Structure of LH 2 of *Rs. molischianum*



molecular replacement



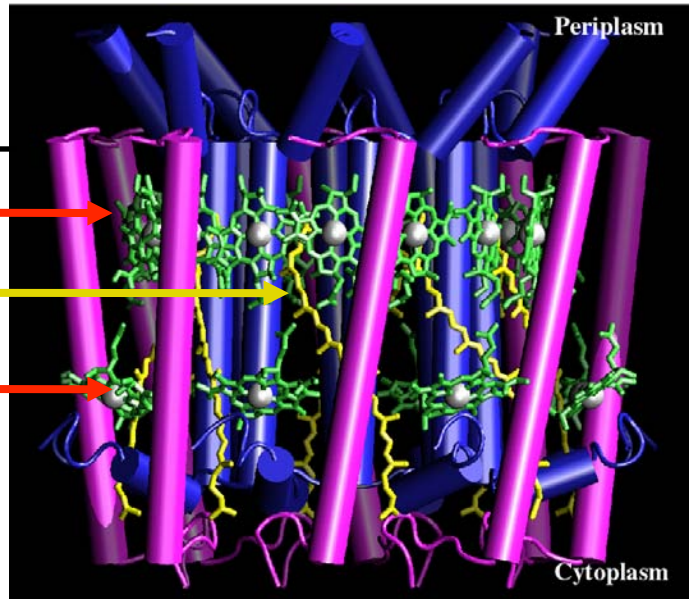


B850 band

B500 band

B800 band

optical spectrum

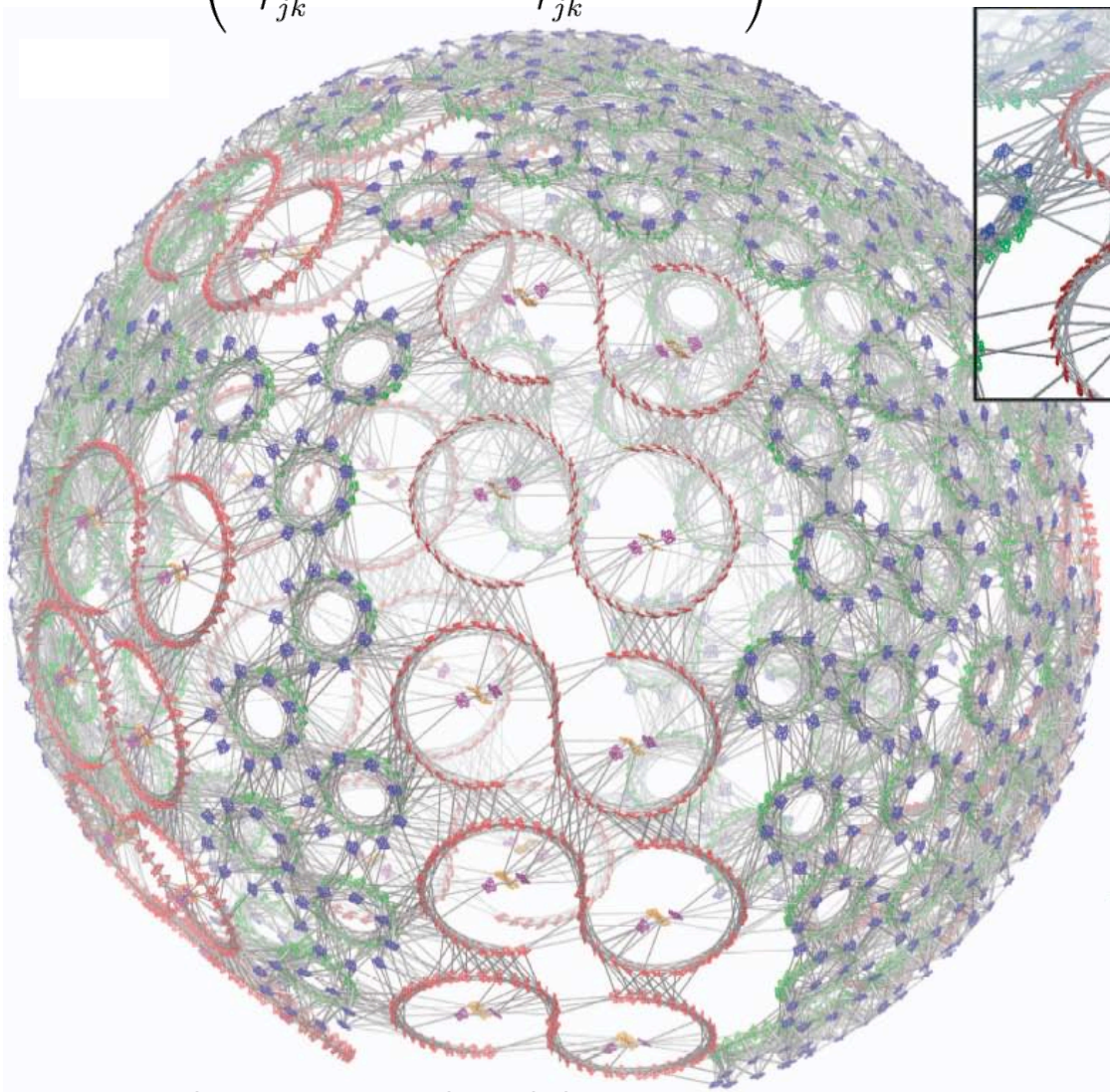


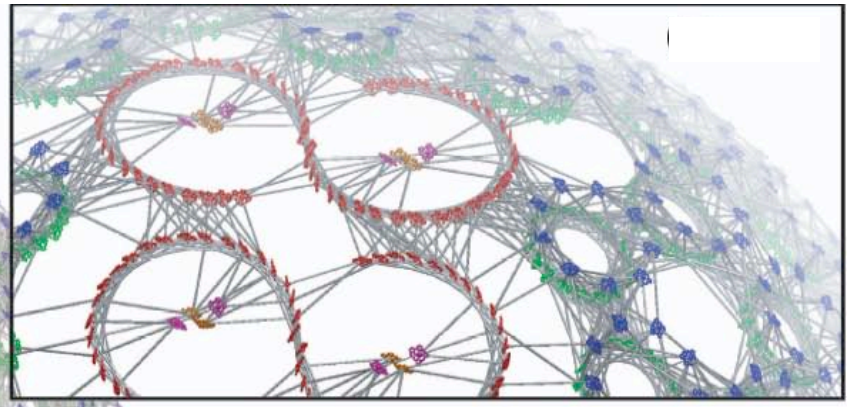
Koepke et al., Structure, **4**, 581 (1996)

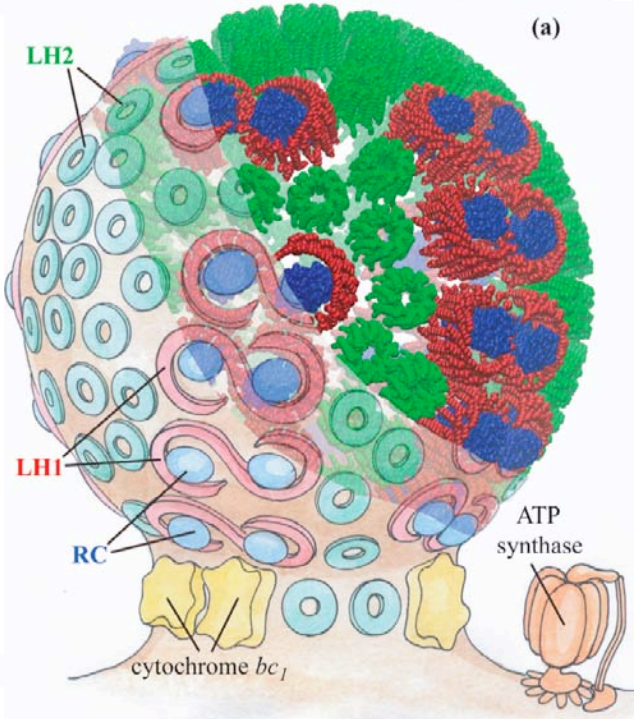
The “Physics” of Light Harvesting in the Chromatophore

Calculated Energy Transfer Rates Determine Optimal Placement of Proteins in Chromatophore

$$W_{jk} = C\left(\frac{\vec{d}_j \cdot \vec{d}_k}{{r_{jk}}^3} - \frac{3(\vec{r}_{jk} \cdot \vec{d}_j)\,(\vec{r}_{jk} \cdot \vec{d}_k)}{{r_{jk}}^5}\right)$$ links: induced dipole - induced dipole interaction







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Acknowledgements

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National Center for Research Resources

VMD team
J. Stone (leader)
D. Hardy
B. Isralewitz
K. Vandivoort