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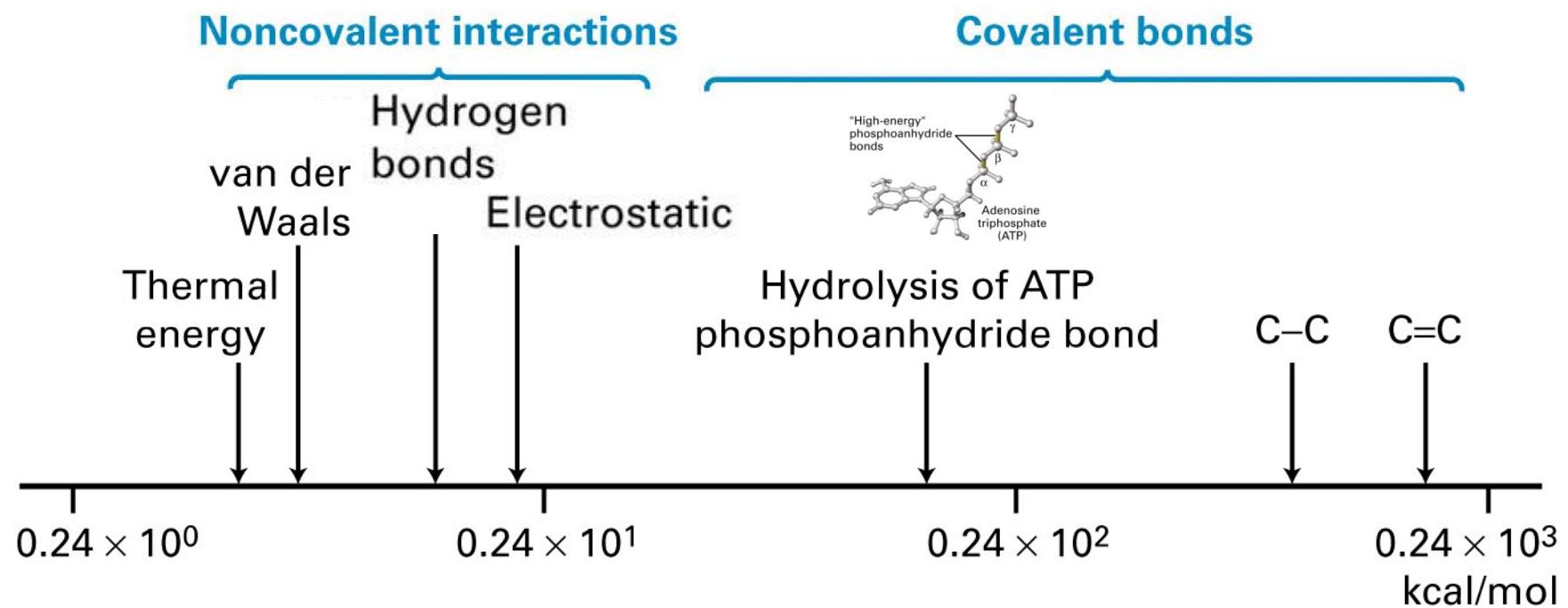
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Y.T.Lin's Presentation

Lecture

Noncovalent Interactions

Noncovalent Interactions



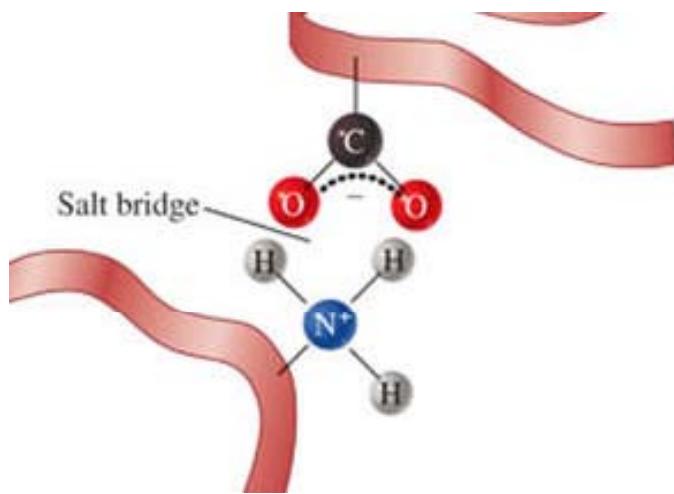
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Noncovalent Interactions

- Charge-Charge Interactions
- Charge-Dipole Interactions
- Dipole-Dipole Interactions
- Charge-induced dipole Interactions
- Hydrogen Bonds
- van der Waals Interactions

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Charge-Charge Interactions



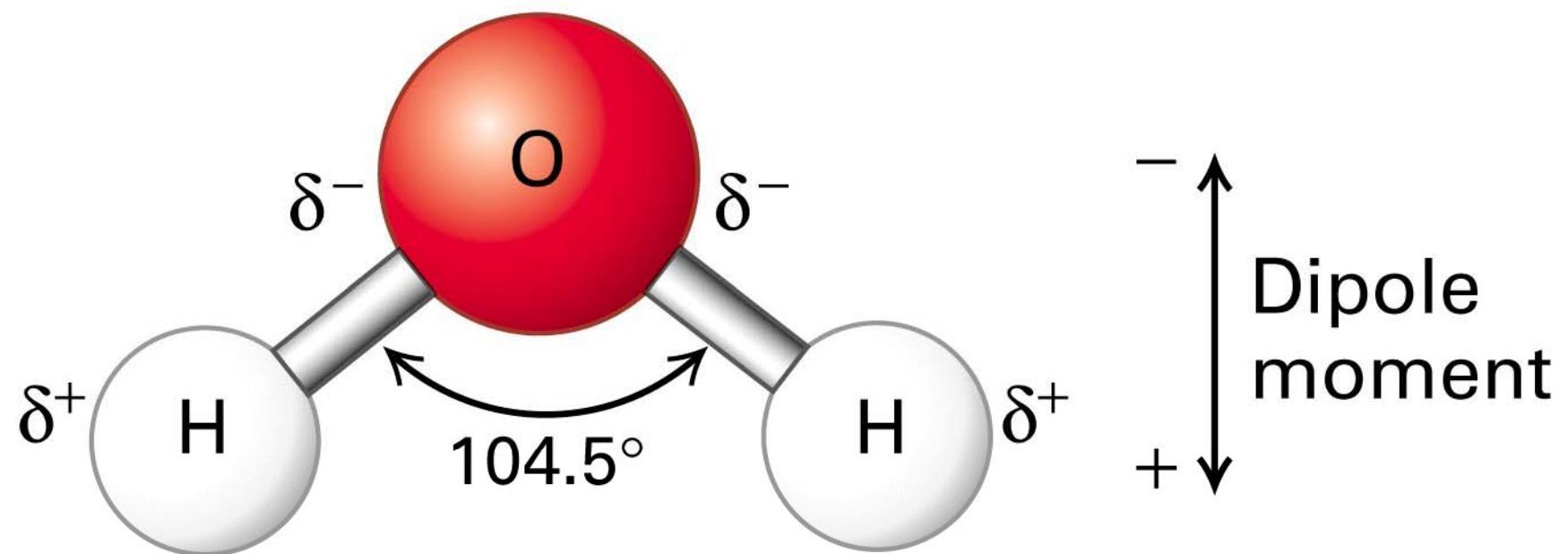
$$Force = k_c \times \frac{q_1 \times q_2}{r_{12}^2}$$

$$Potential = k_c \times \frac{q_1 \times q_2}{r_{12}}$$



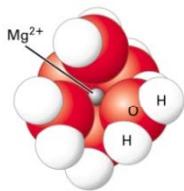
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Dipole moment



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Ion-Dipole Interaction



$$Potential = k_{ion-dipole} \times \frac{q \times u}{r^2}$$

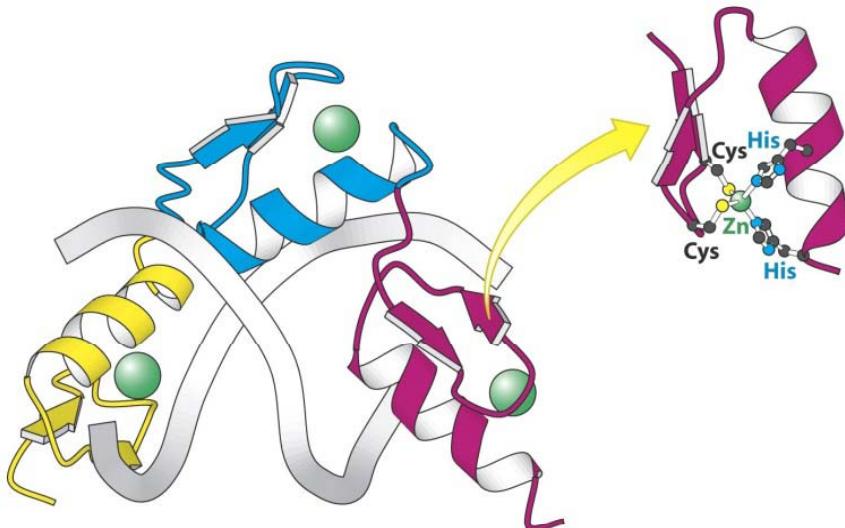
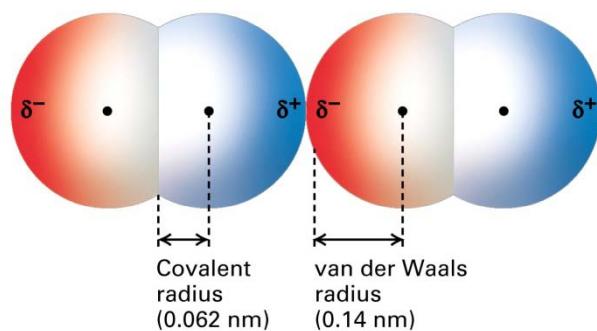


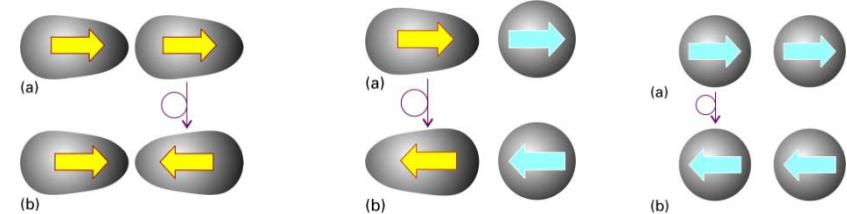
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Dipole-Dipole Interactions

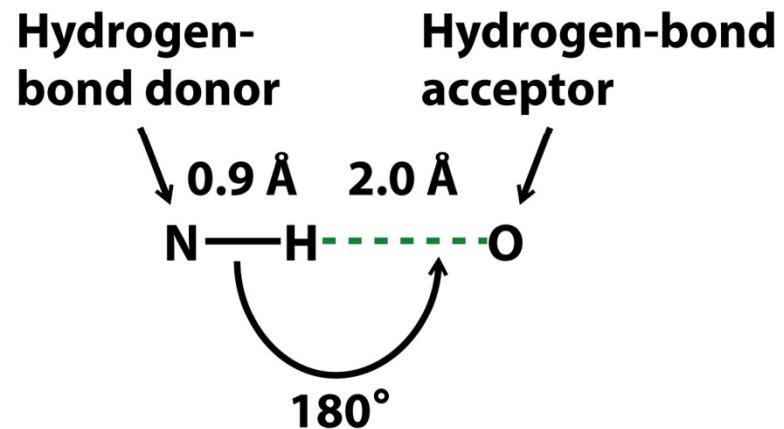
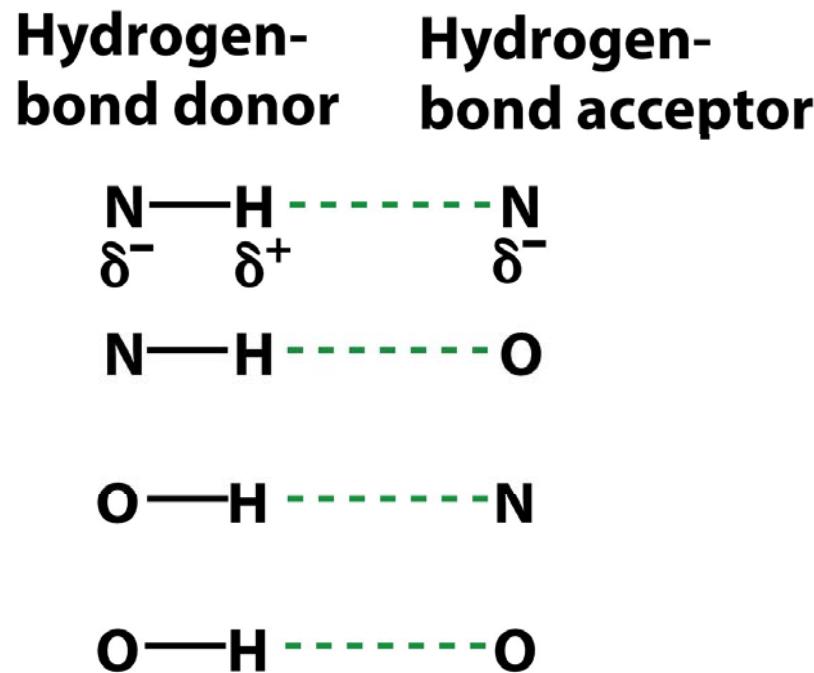


$$\text{Potential} = k_{\text{dipole-dipole}} \frac{\mathbf{u}_1 \times \mathbf{u}_2}{r^3}$$

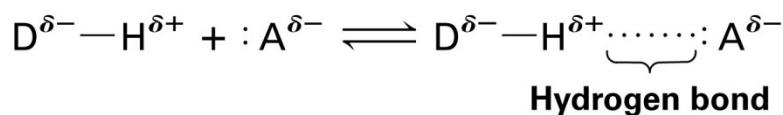
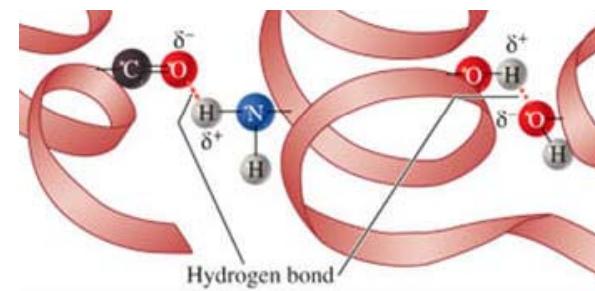


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Hydrogen Bonds

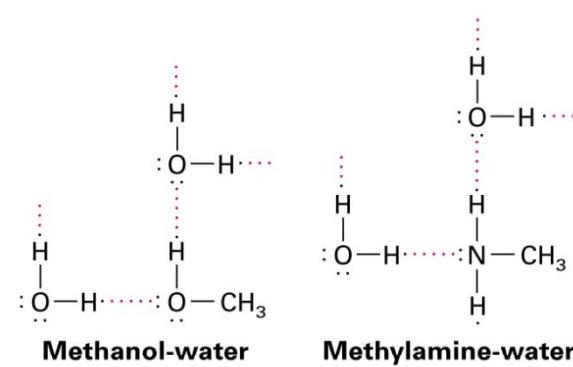
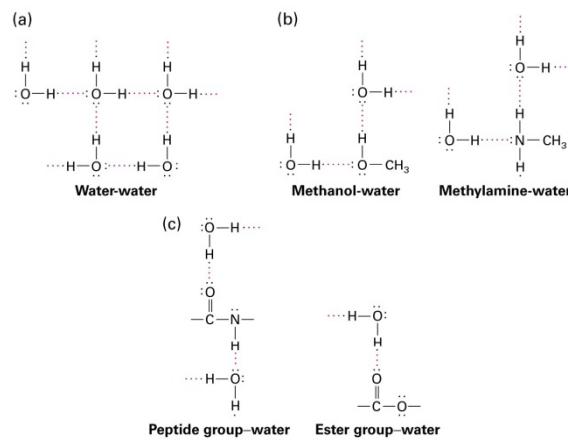
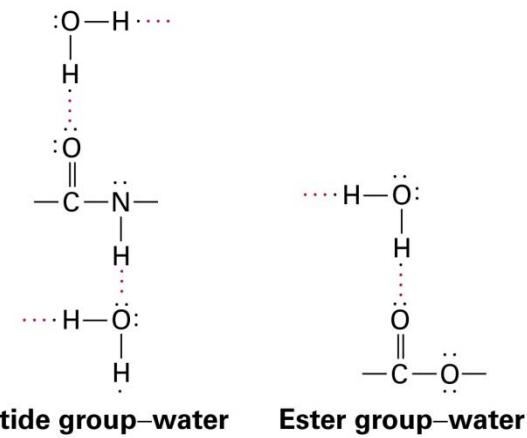
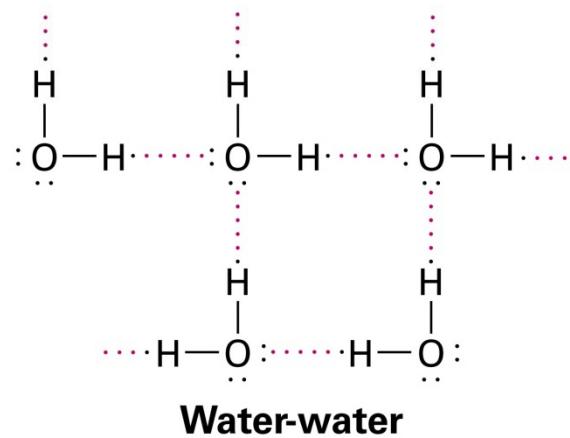


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Hydrogen Bonds with Water



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Charge-Induced Dipole Interaction

$$Potential = k_{ion-induced-dipole} \times \frac{q}{r^4}$$

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van der Waals Interactions

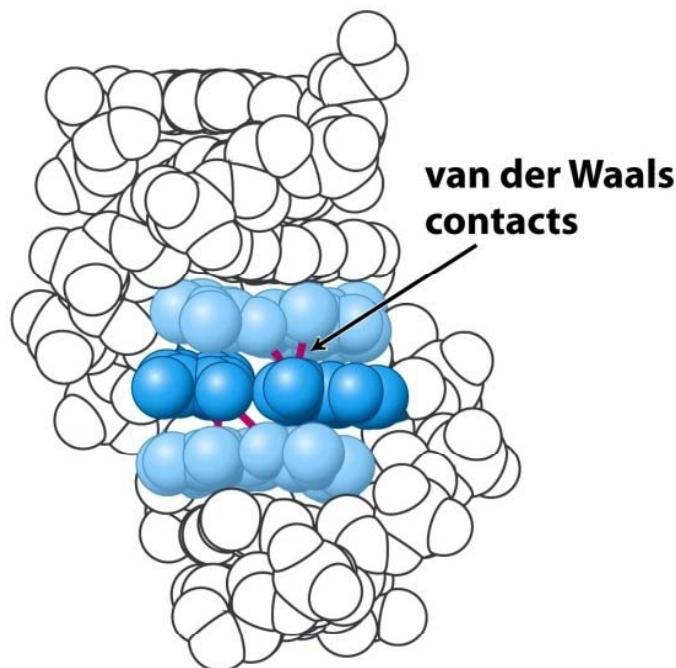


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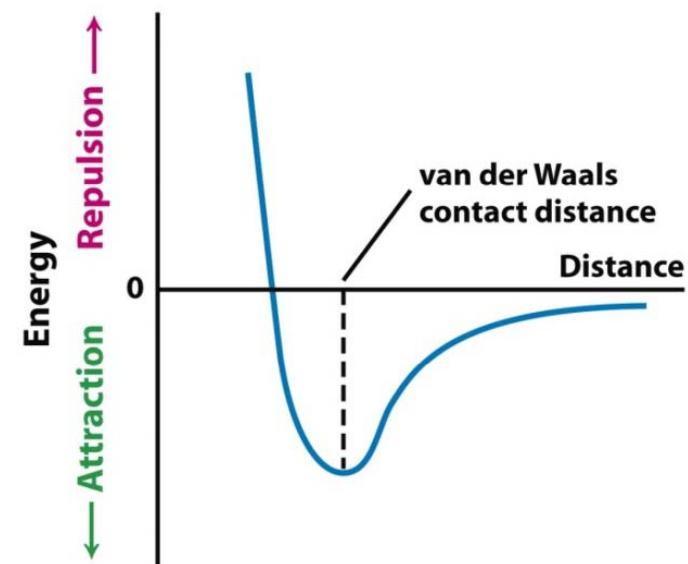
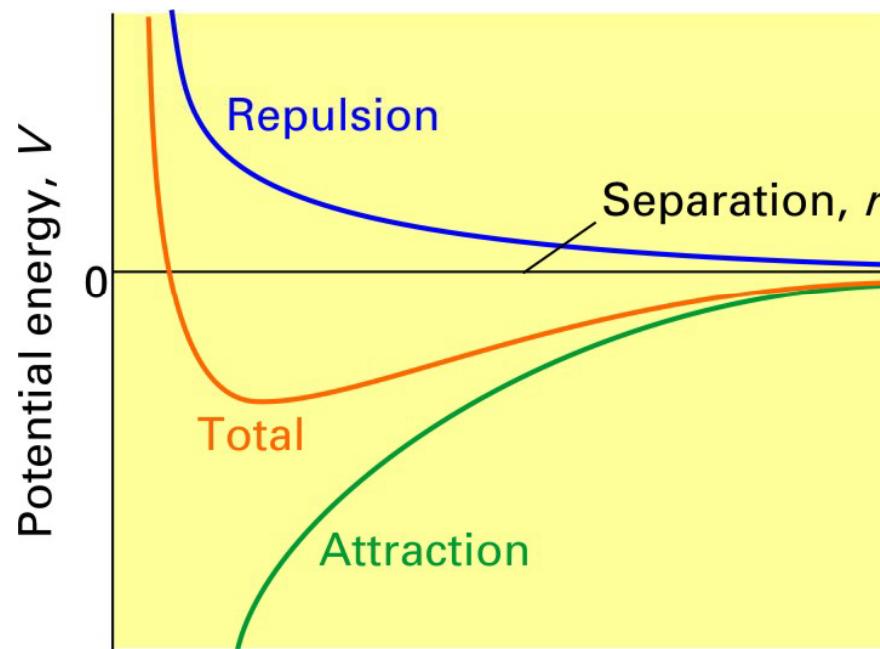


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van der Waals Interactions

$$Potential = k_{van-der-Waals} \left\{ \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right\}$$



Presentation

Distance Dependence

ion type	Distance dependence of potential energy	Typical energy (kJ mol ⁻¹)	Comment
ion	$1/r$	250.0	Only between ions
dipole	$1/r^2$	15.0	
lipole	$1/r^3$	2.0	Between stationary molecules
	$1/r^6$	0.3	Between rotating molecules
duced dipole	$1/r^4$		
ion	$1/r^6$	2.0	Between all types of molecules and ions
ion	$1/r^{12}$	2.0	Between all types of molecules and ions

✓ a hydrogen bond X-H ... Y is typically 20 kJ mol⁻¹ and occurs on contact for X, Y = N, O, or F

Self-Assembly

- By non-covalent interactions.

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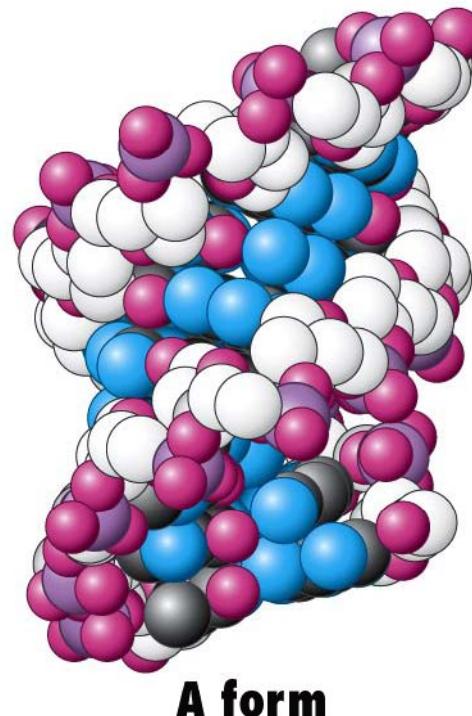
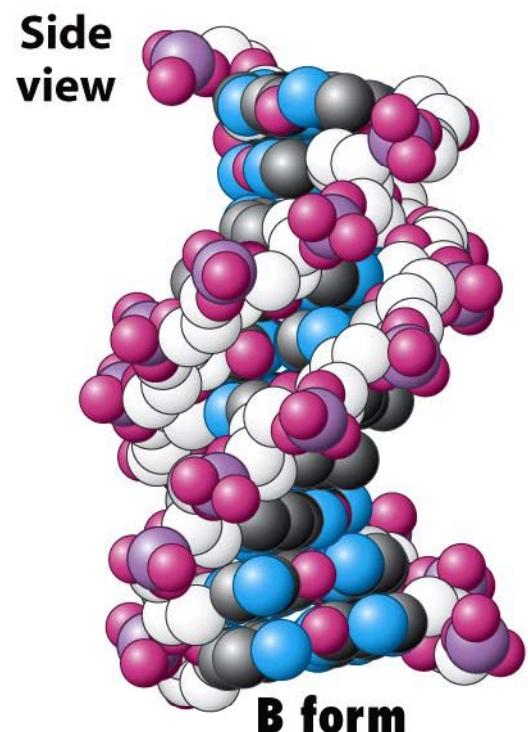
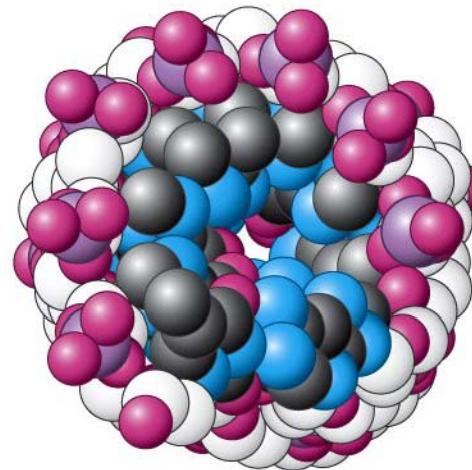
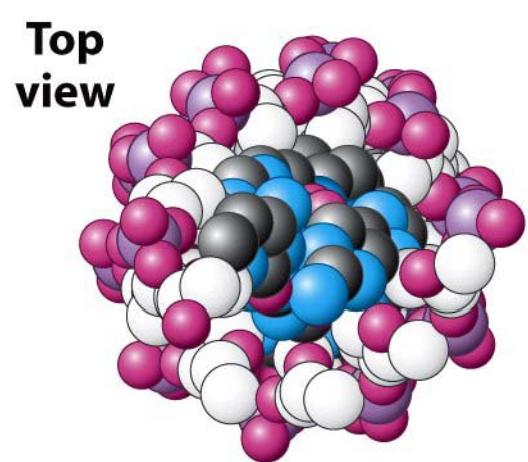
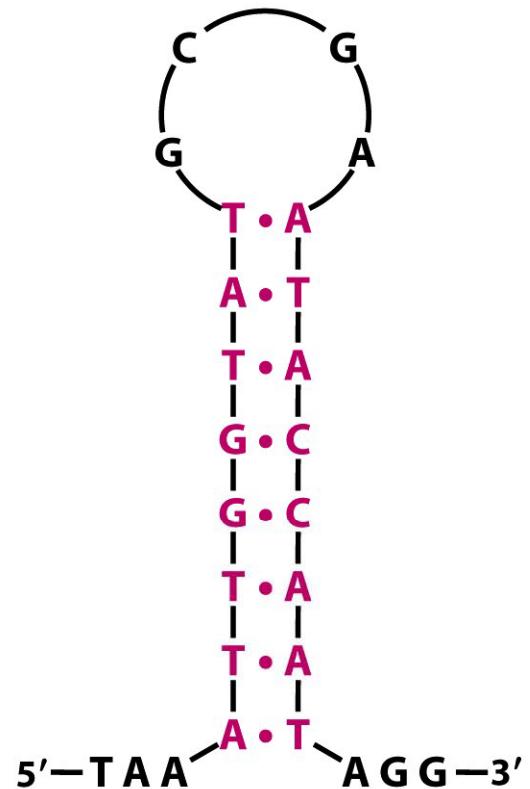


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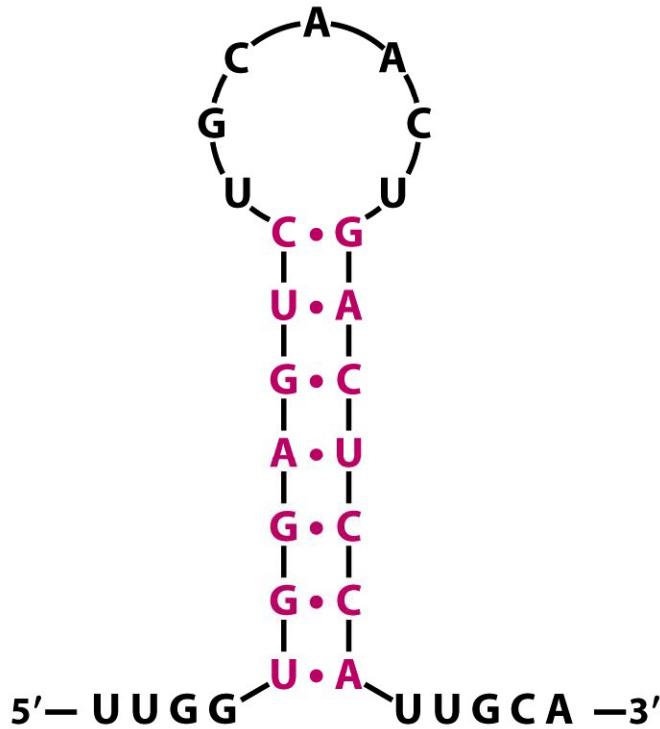
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DNA molecule



RNA molecule

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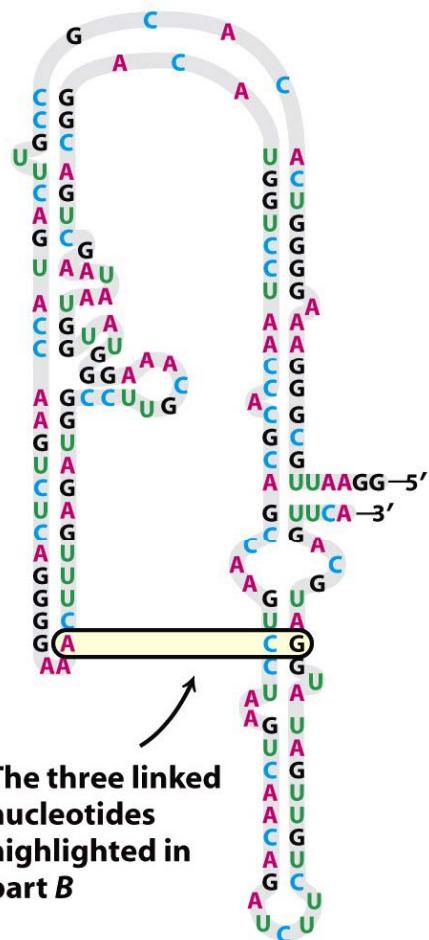


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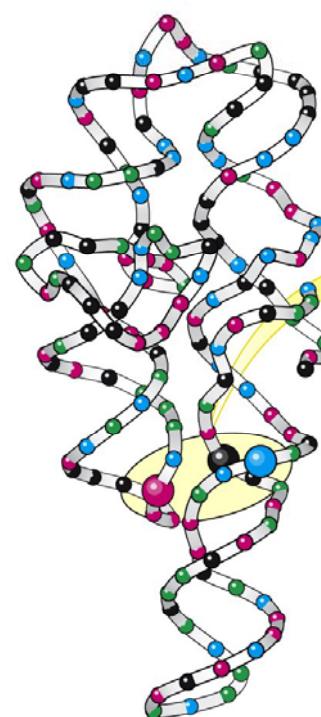
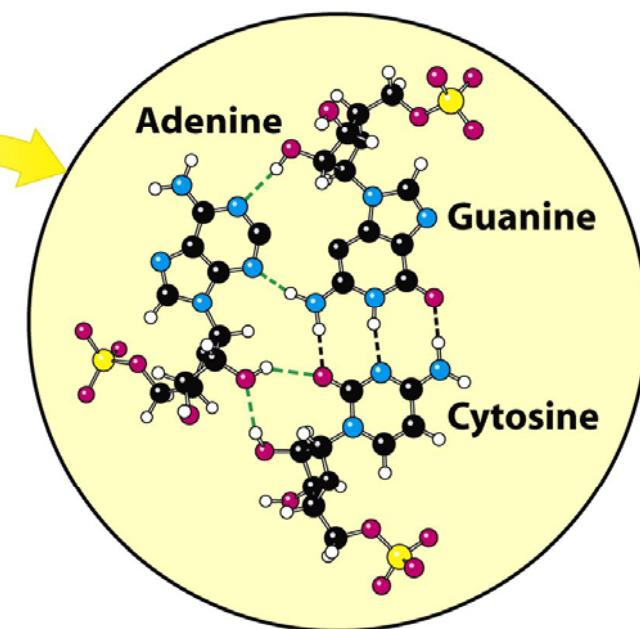


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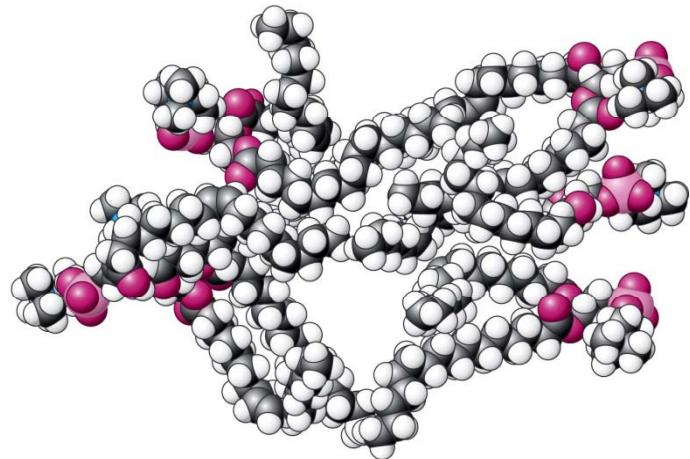


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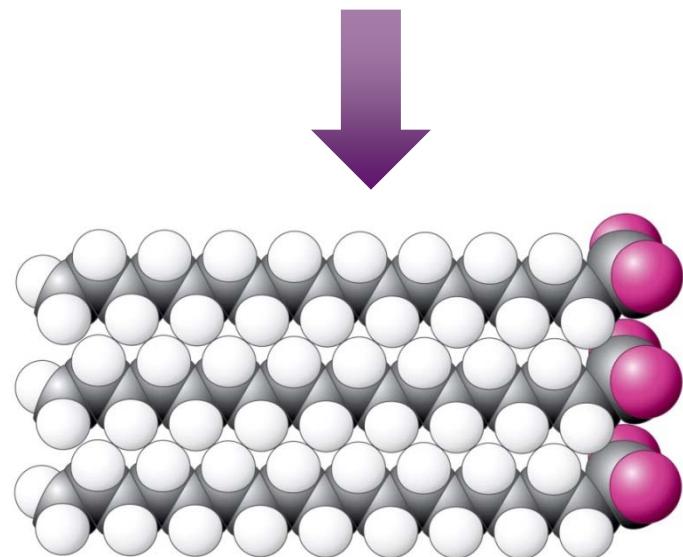
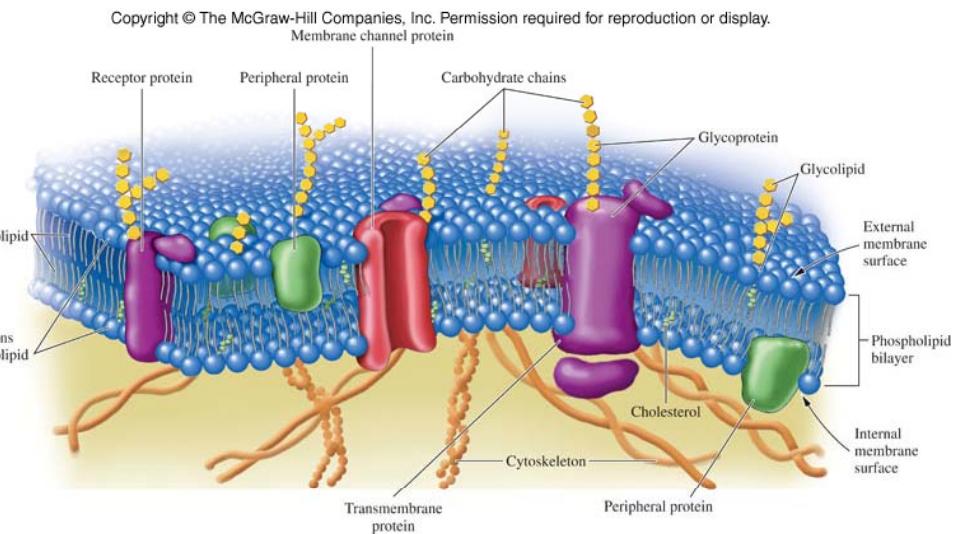
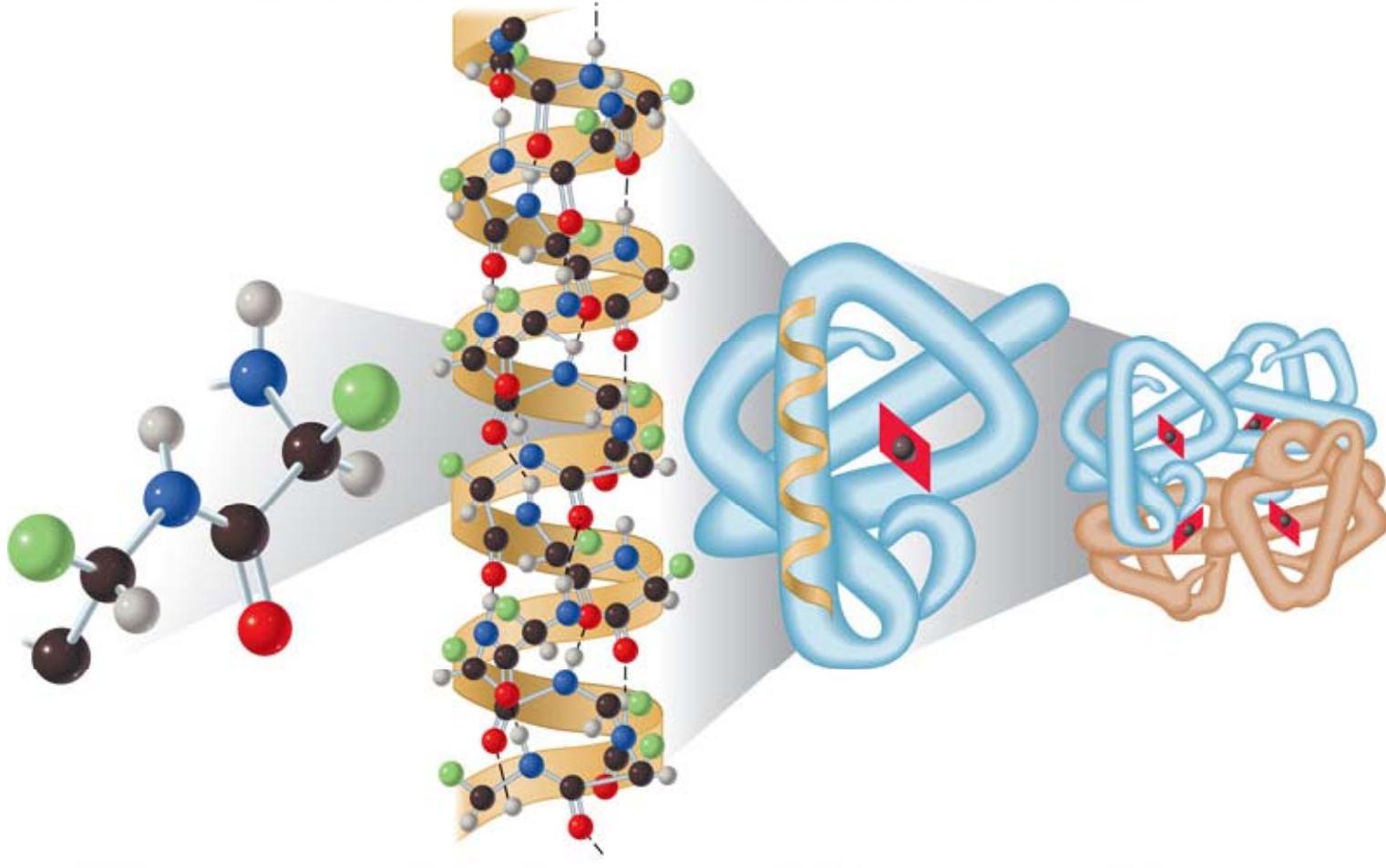


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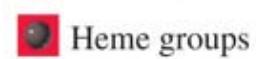


(a) Primary structure

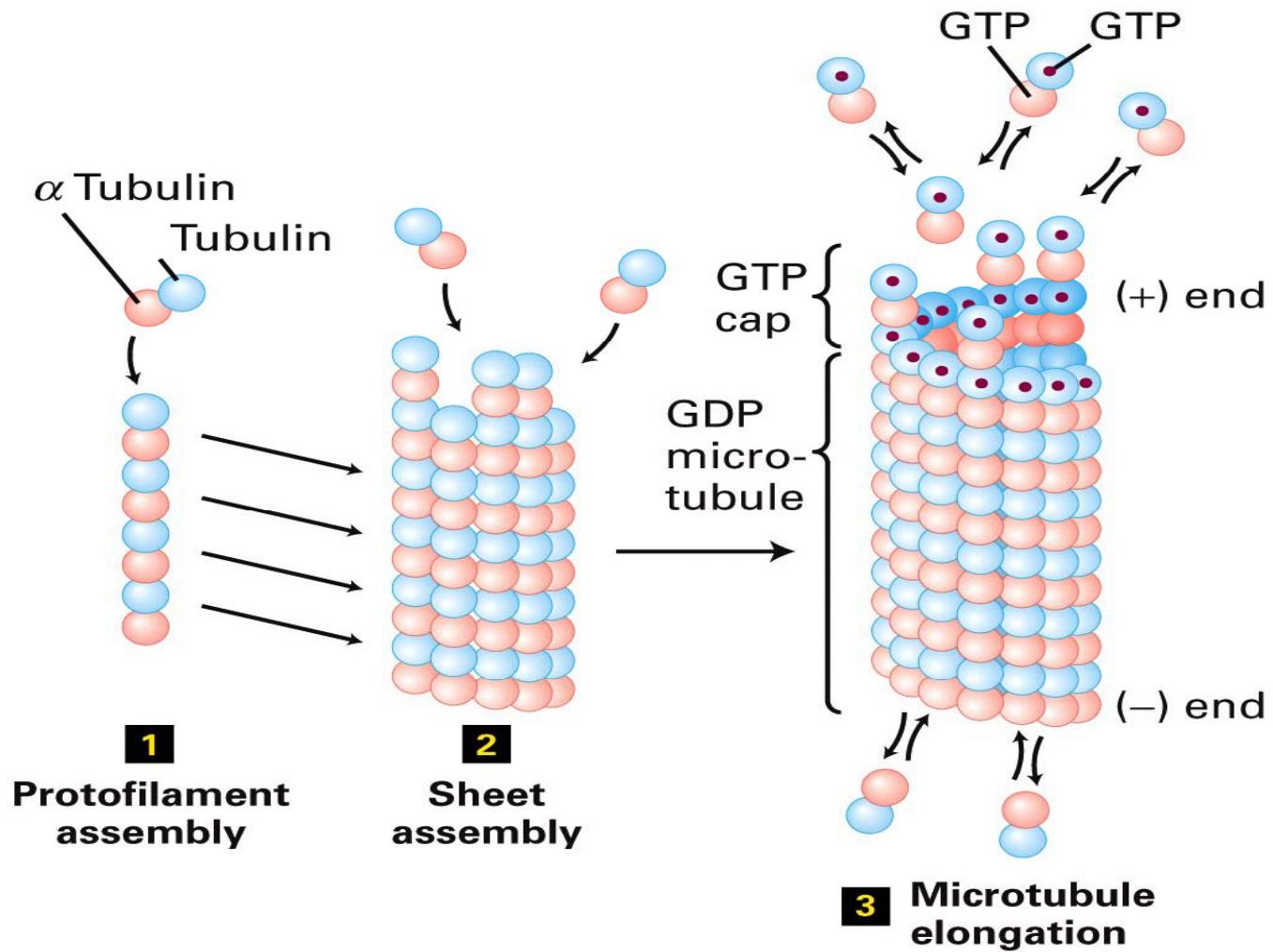
(b) Secondary structure

(c) Tertiary structure

(d) Quaternary structure



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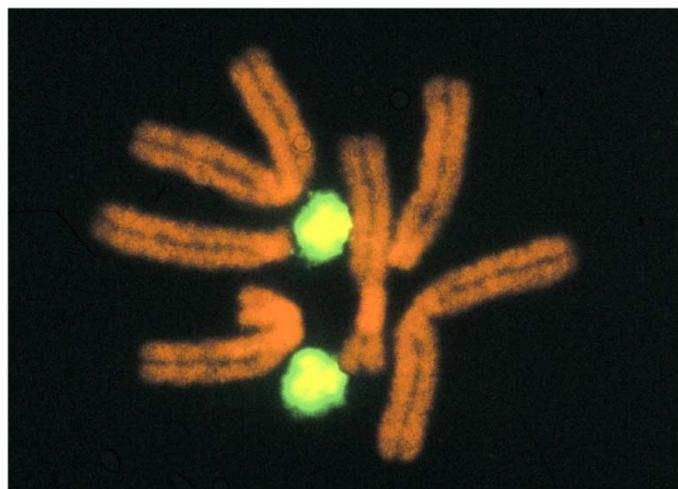


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