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SMR: 1643/8

WINTER COLLEGE ON OPTICS ON OPTICS AND PHOTONICS IN NANOSCIENCE AND NANOTECHNOLOGY

(7 - 18 February 2005)

"Biophotonics at the Nanoscale" - II

presented by:

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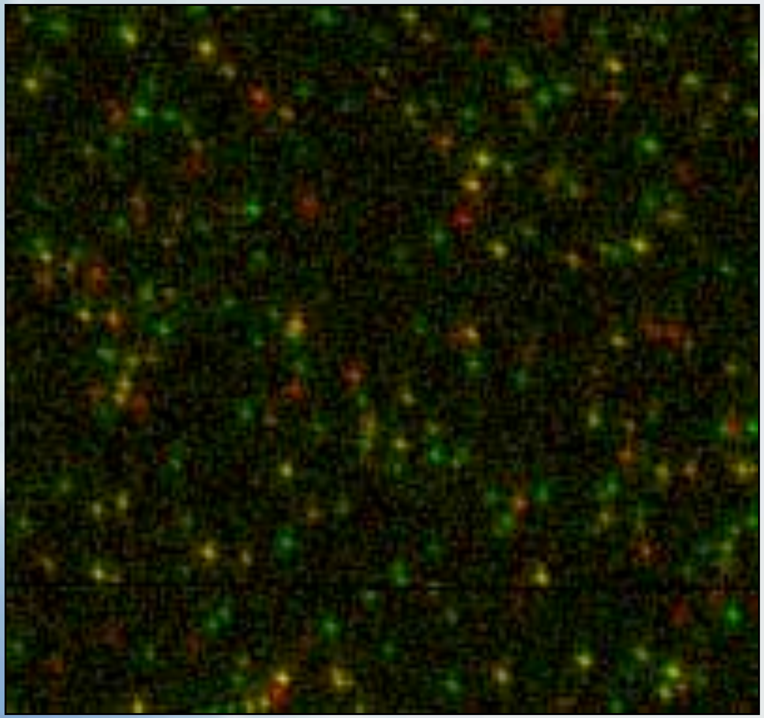
SP FRET

(single-pair fluorescence resonance energy transfer)



www.nano-optics.org

Lukas Novotny

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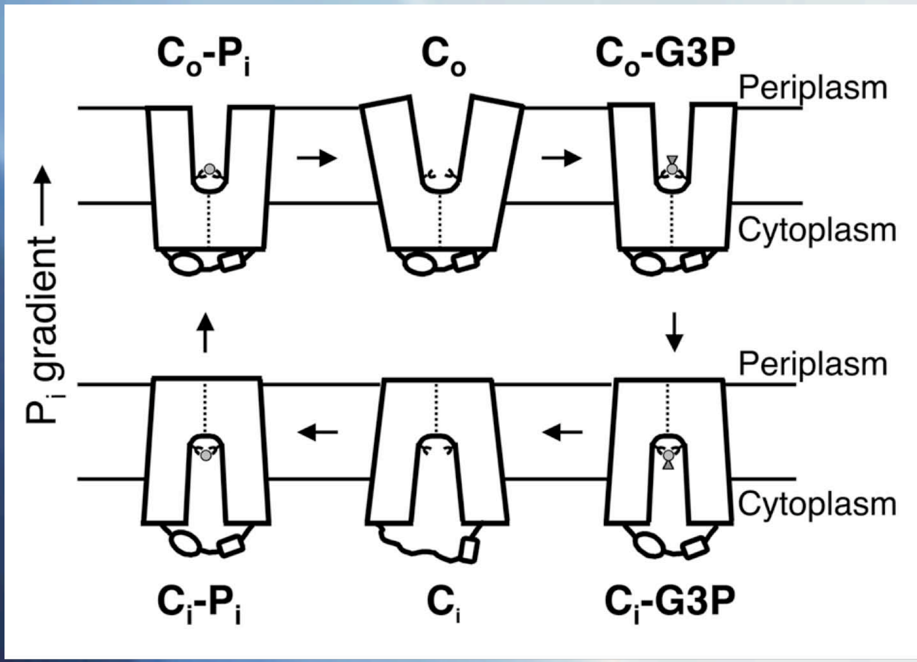
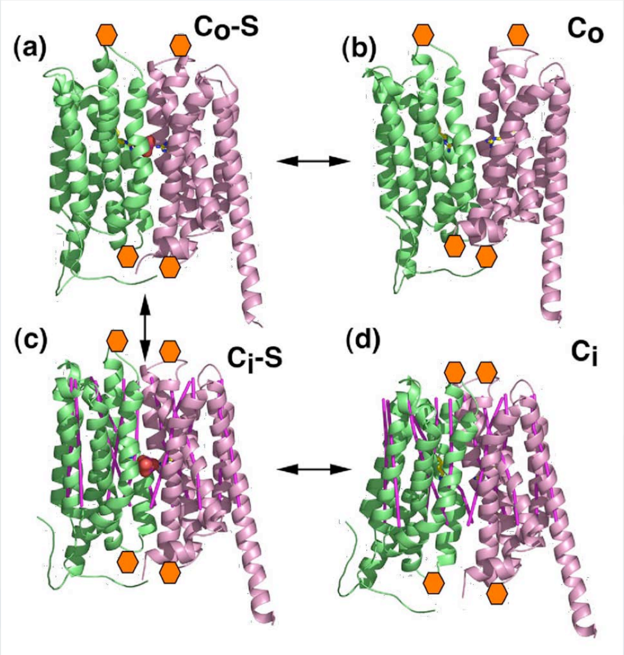
EXAMPLE: ROCKERSWITH MODEL FOR GlpT





Reaction cycle of substrate translocation: Proposed single-binding-site, alternating-access mechanism with a rocker-switch type of movement . Positions of Arg45 and Arg269 are indicated. P_i is represented by a small disk, and the G3P molecule as a small disk and a triangle.

TEXTBOOK (Cambridge Univ. Press)

PRINCIPLES
OF
NANO-OPTICS

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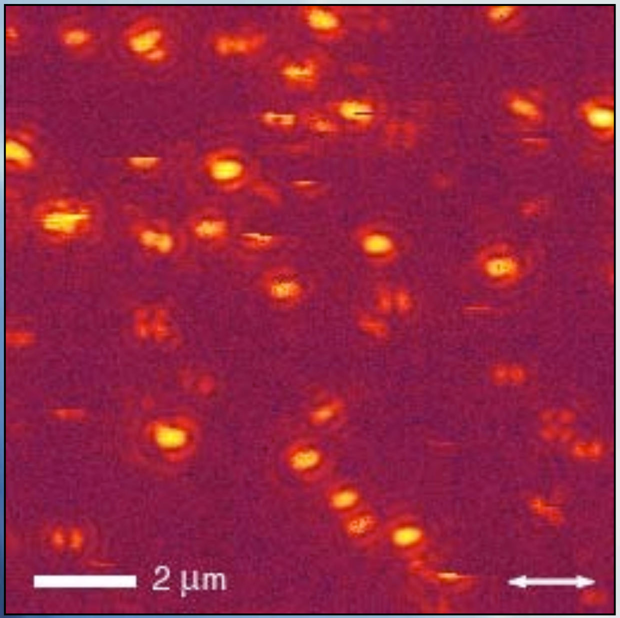
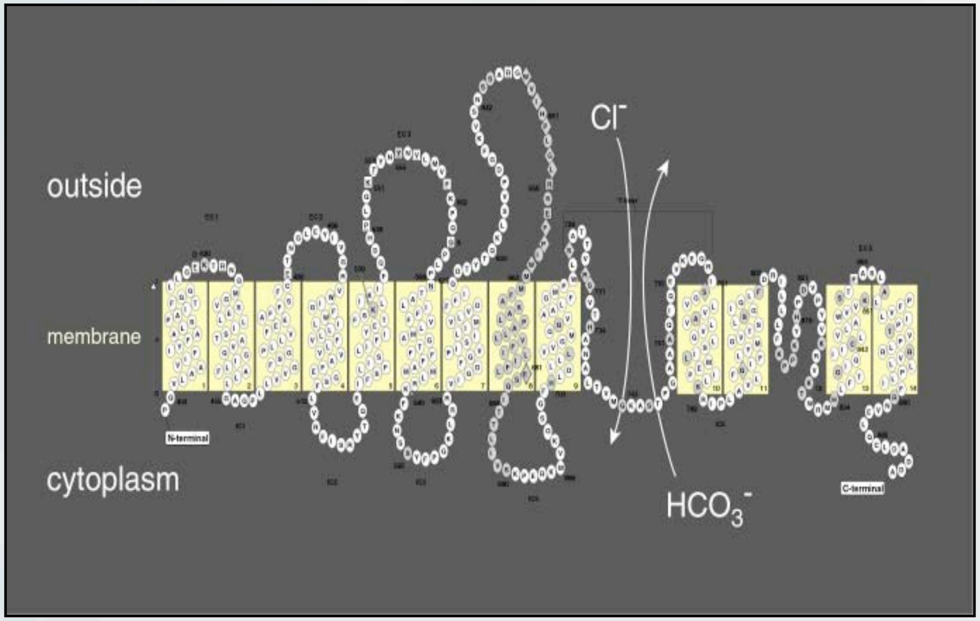
University of Basel, Basel, Switzerland

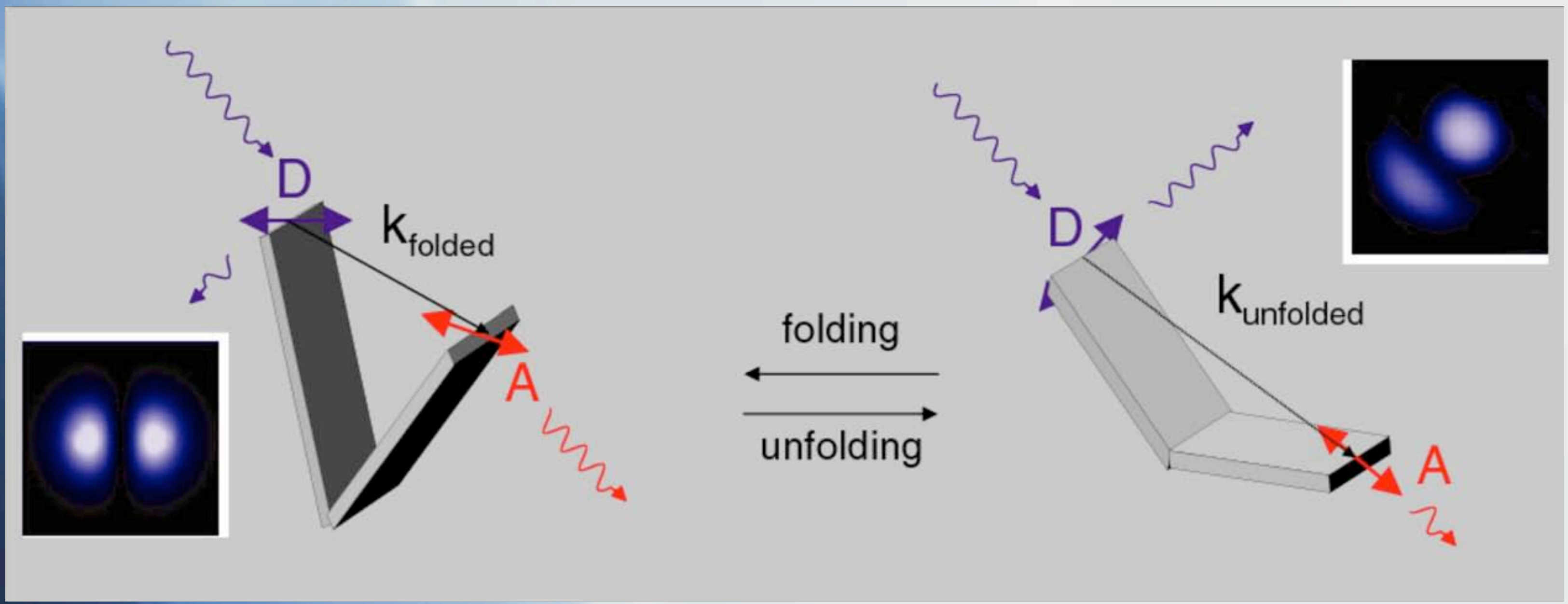
CONFORMATIONAL STATES OF AE1





Collaboration with Prof. P. Knauf (Biochemistry, Rochester)

FOERSTER ENERGY TRANSFER



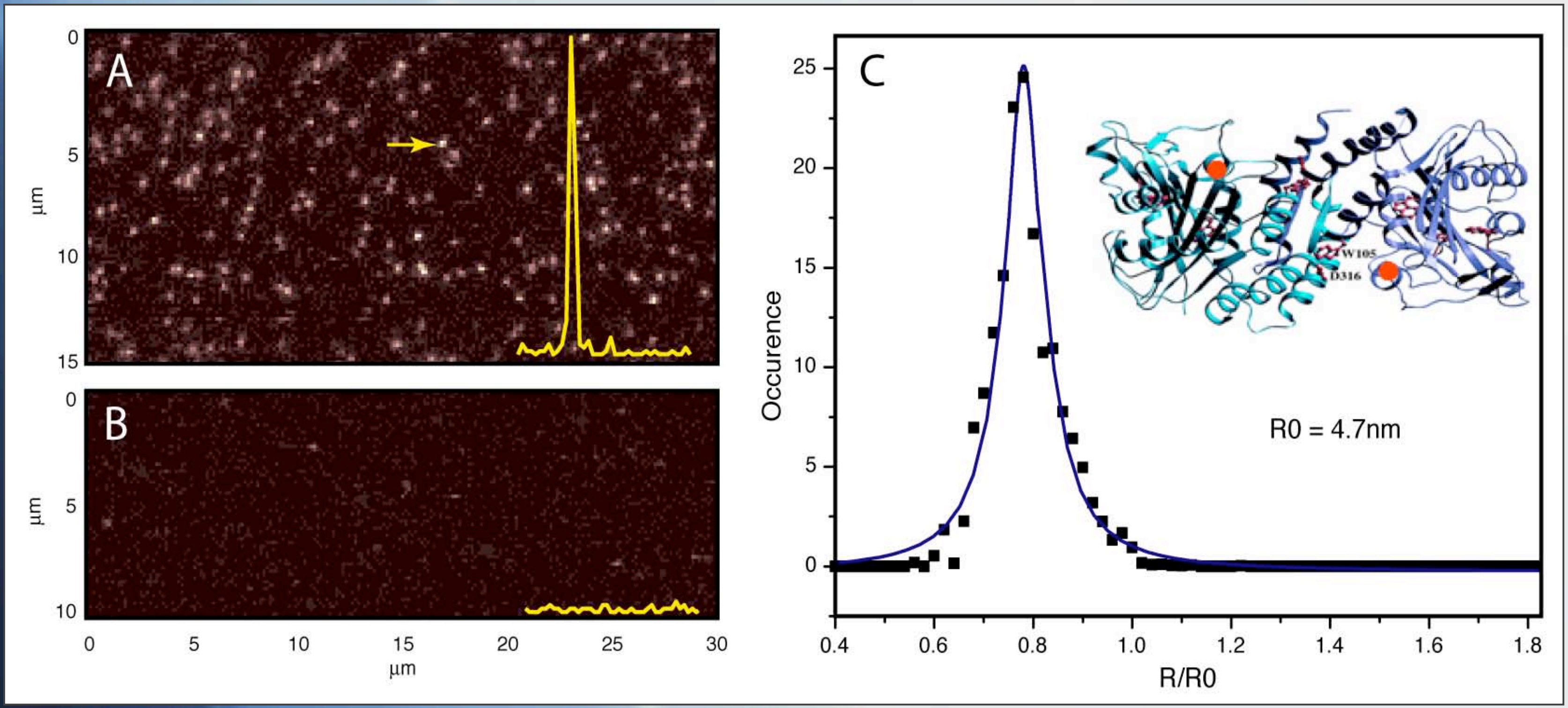
$$R_o^6 = \frac{9000(\ln 10)\kappa^2 \phi_D}{128\pi^2 N_{av}\ n^4} \int_0^{\infty} F_D(\lambda)\varepsilon_A(\lambda)\lambda^4 d\lambda$$

$$\kappa^2 = [\mathbf{n}_A \, . \, \mathbf{n}_D - 3(\mathbf{n}_R \, . \, \mathbf{n}_D)(\mathbf{n}_R \, . \, \mathbf{n}_A)]^2$$

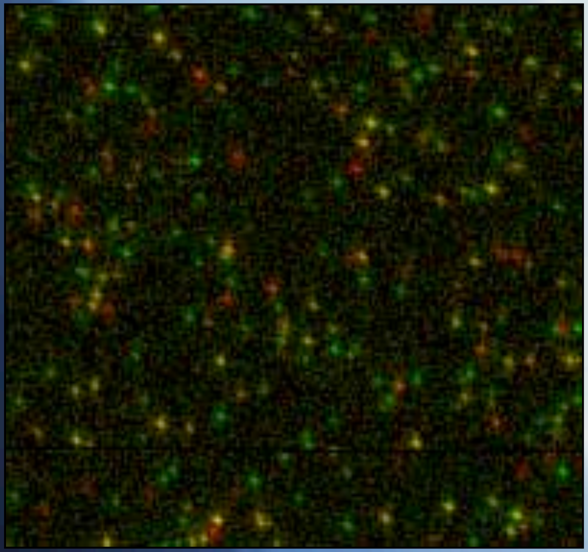
FOERSTER WHO ?

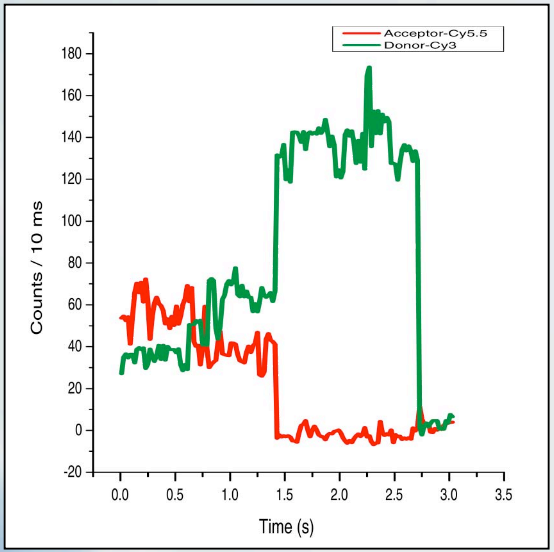
Robert S. Knox (left) and Theodore Foerster (right) preparing for mechanical energy transfer. Springwater, NY, August 1973.

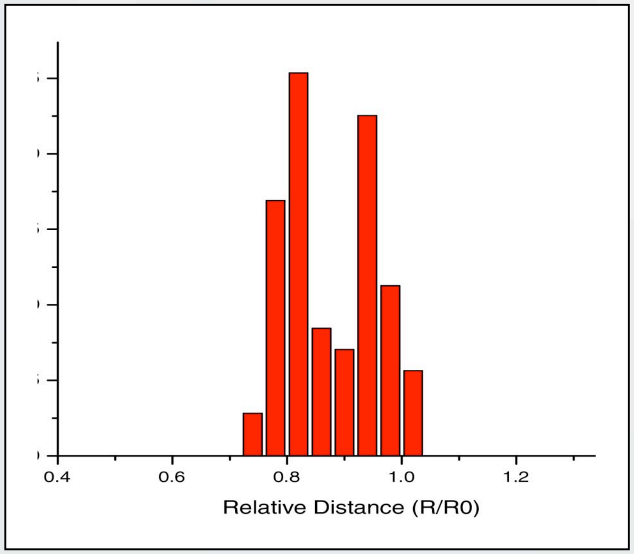
CYTOPLASMIC DOMAIN OF AE1 (CDB3)



STATIC CONFORMATIONS OF AE1







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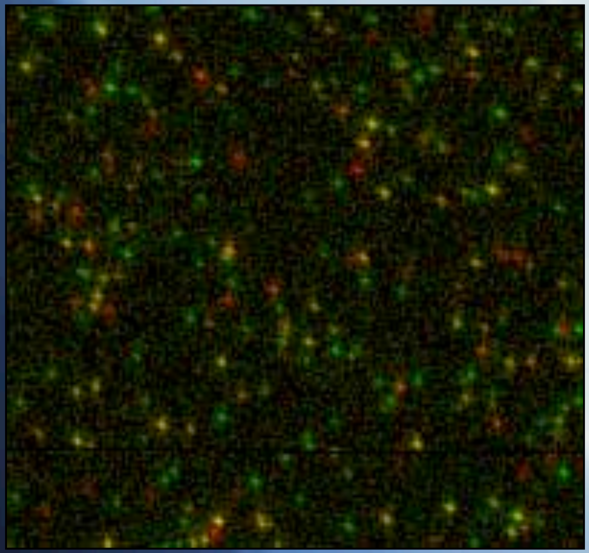
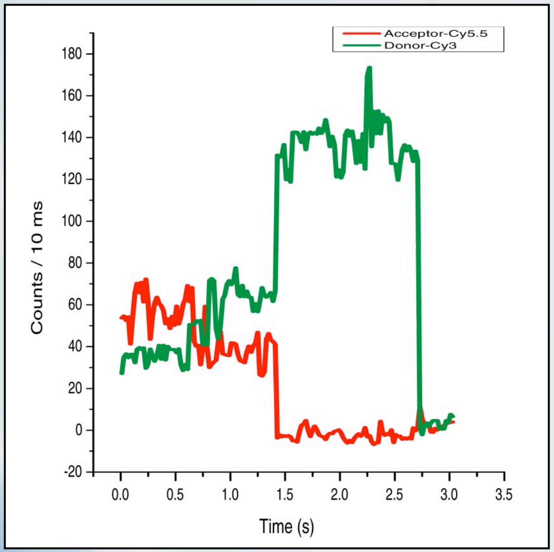
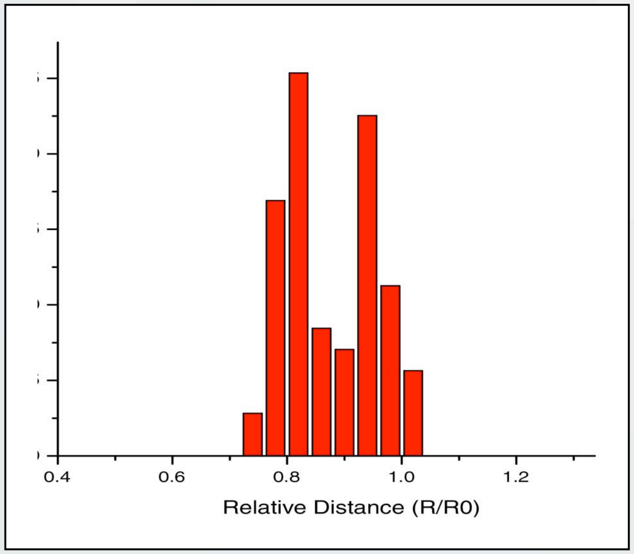
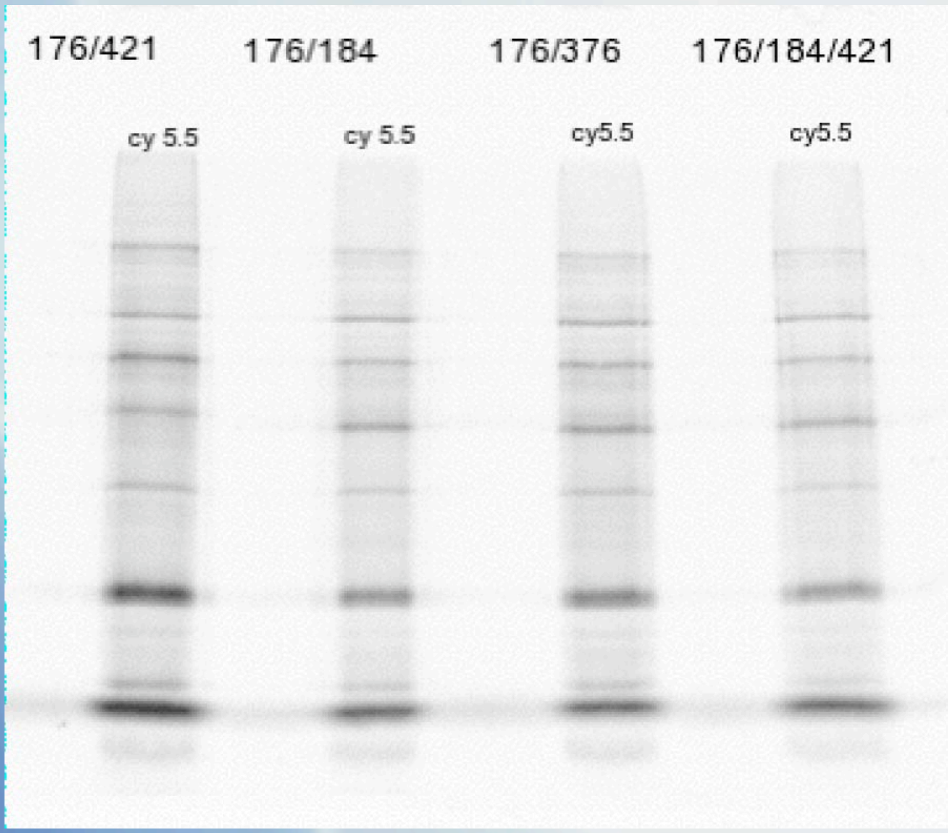


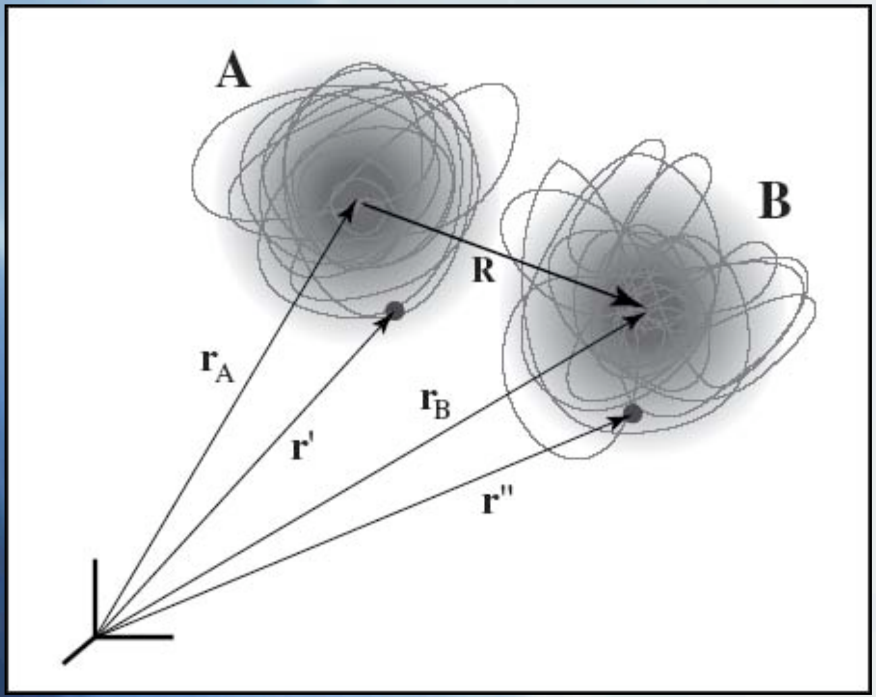




PROBLEM: PURIFICATION



ENERGY TRANSFER THEORY

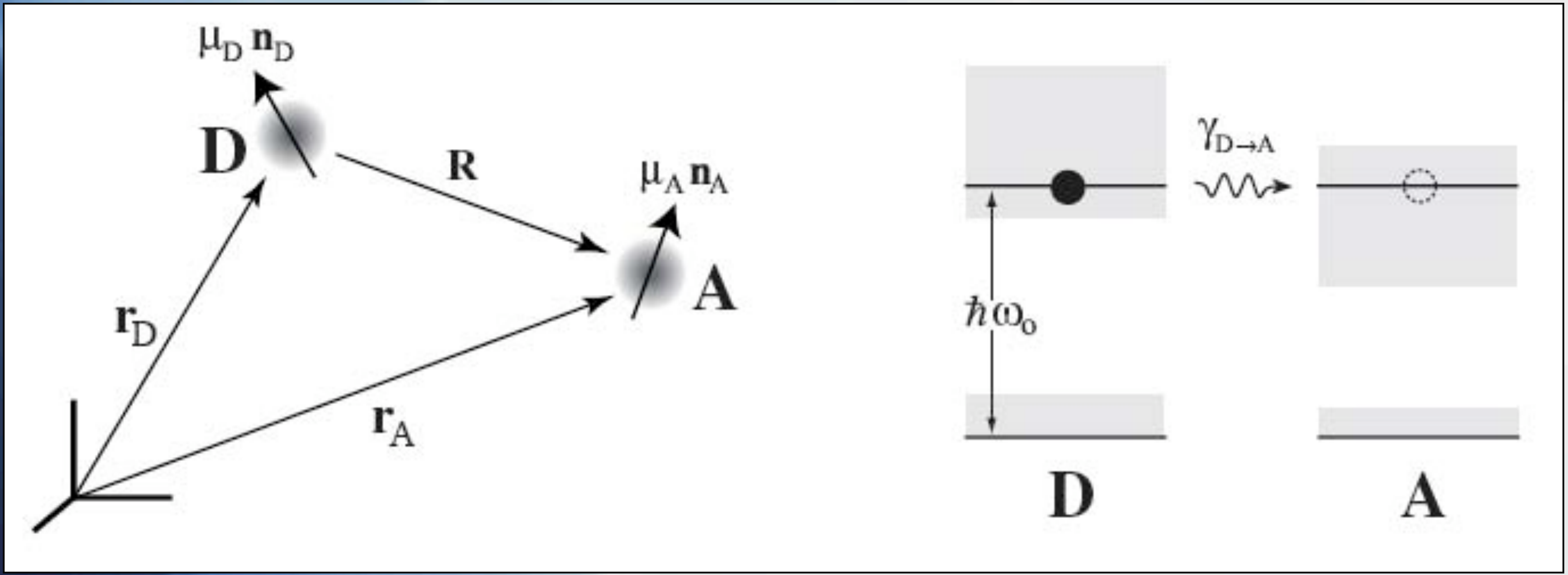


$$q_A = \int \rho_A(\mathbf{r}')\, dV'$$

$$\mu_A = \int \rho_A(\mathbf{r}')\,(\mathbf{r}' - \mathbf{r}_A)\, dV'$$

$$V_{AB}(\mathbf{R}) = \frac{1}{4\pi\varepsilon_o}\Big[\frac{q_A q_B}{R} + \frac{q_A\, \boldsymbol{\mu}_B\cdot\mathbf{R}}{R^3} - \frac{q_B\, \boldsymbol{\mu}_A\cdot\mathbf{R}}{R^3} + \frac{R^2\, \boldsymbol{\mu}_A\cdot\boldsymbol{\mu}_B - 3\,(\boldsymbol{\mu}_A\cdot\mathbf{R})\,(\boldsymbol{\mu}_B\cdot\mathbf{R})}{R^5} + \dots$$

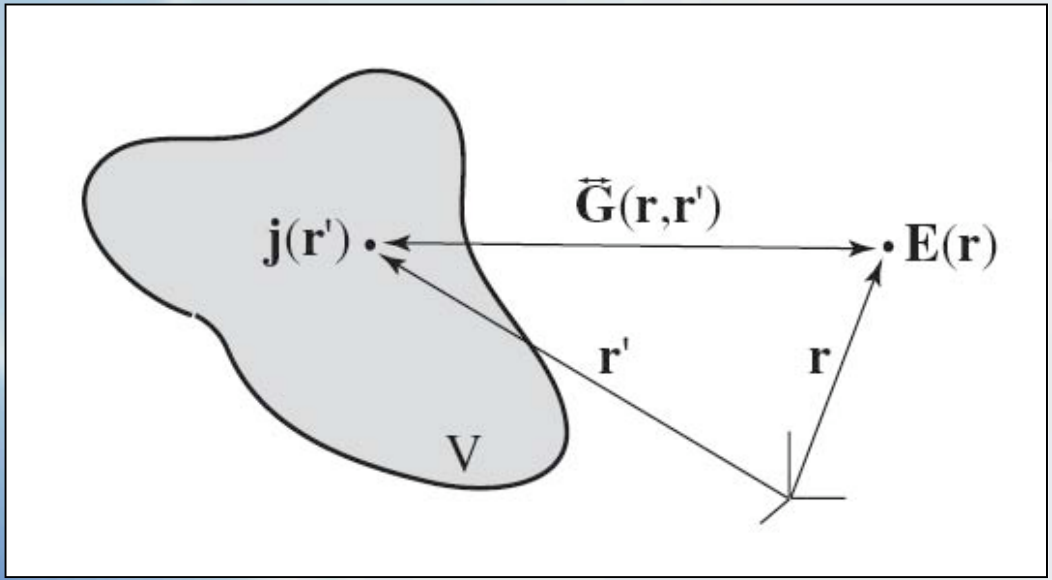
LIMIT: WEAK COUPLING



$$\frac{\gamma_{D\to A}}{\gamma_o} = \frac{P_{D\to A}}{P_o}.$$

$$P_o = \frac{|\mu_D|^2\, n(\omega_o)}{12\pi\,\varepsilon_o\, c^3}\,\omega_o^4$$

GREEN'S FUNCTIONS



$$\mathbf{j}(\mathbf{r}) = -i\omega\mu\,\delta[\mathbf{r}-\mathbf{r}_o]$$

$$\mathbf{E}(\mathbf{r}) = \omega^2\mu_o\mu\,\overleftrightarrow{\mathbf{G}}\,(\mathbf{r},\mathbf{r}')\,\boldsymbol{\mu}$$

POWER TRANSFER

$$P_{D\rightarrow A} \;=\; -\frac{1}{2}\int_{V_A} \mathrm{Re}\{\mathbf{j}_A^* \cdot \mathbf{E}_D\}\, dV$$

For $\mathbf{j}_A = -i\omega_o \boldsymbol{\mu}_A\, \delta(\mathbf{r}-\mathbf{r}_A)$:

$$P_{D\rightarrow A} \;=\; \frac{\omega_o}{2}\, \mathrm{Im}\{\boldsymbol{\mu}_A^* \cdot \mathbf{E}_D(\mathbf{r}_A)\}$$

Induced dipole $\boldsymbol{\mu}_A \;=\; \overset{\leftrightarrow}{\alpha}_A\, \mathbf{E}_D(\mathbf{r}_A)$ with $\overset{\leftrightarrow}{\alpha}_A = \alpha_A\, \mathbf{n}_A \mathbf{n}_A$:

$$P_{D\rightarrow A} \;=\; \frac{\omega_o}{2}\, \mathrm{Im}\{\alpha_A\} \left|\mathbf{n}_A \cdot \mathbf{E}_D(\mathbf{r}_A)\right|^2$$

ABSORPTION CROSS-SECTION

$$\sigma(\omega_o) \;=\; \frac{\langle P(\omega_o)\rangle}{I(\omega_o)}$$

$$\sigma(\omega_o) \;=\; \frac{(\omega_o/2)\,\mathrm{Im}\{\alpha(\omega_o)\}\,\langle|\mathbf{n_p}\cdot\mathbf{E}_D|^2\rangle}{(1/2)\,(\varepsilon_o/\mu_o)^{1/2}\,n(\omega_o)\,|\mathbf{E}_D|^2} \;=\; \frac{\omega_o}{3}\sqrt{\frac{\mu_o}{\varepsilon_o}}\,\frac{\mathrm{Im}\{\alpha(\omega_o)\}}{n(\omega_o)}$$

$$P_{D\to A} \;=\; \frac{3}{2}\sqrt{\frac{\varepsilon_o}{\mu_o}}\,n(\omega_o)\,\sigma_A(\omega_o)\,\Big|\mathbf{n}_A\cdot\mathbf{E}_D(\mathbf{r}_A)\Big|^2$$

FIELD OF DONOR EVALUATED AT ACCEPTOR

$$\mathbf{E}_D(\mathbf{r}_A) \;=\; \omega_o^2\,\mu_o\,\overleftrightarrow{\mathbf{G}}(\mathbf{r}_D,\mathbf{r}_A)\,\boldsymbol{\mu}_D$$

Short-hand:

$$T(\omega_o) \;=\; 16\pi^2 k^4 R^6 \left|\mathbf{n}_A\cdot\overleftrightarrow{\mathbf{G}}(\mathbf{r}_D,\mathbf{r}_A)\,\mathbf{n}_D\right|^2$$

where $R = |\mathbf{r}_D - \mathbf{r}_A|$

$k = (\omega_o/c)\,n(\omega_o)$.

$$\frac{\gamma_{D\to A}}{\gamma_o} \;=\; \frac{9c^4}{8\pi R^6}\,\frac{\sigma_A(\omega_o)}{n^4(\omega_o)\,\omega_o^4}\,T(\omega_o) \;=\; \frac{9c^4}{8\pi R^6}\int_0^\infty \frac{\delta(\omega-\omega_o)\,\sigma_A(\omega)}{n^4(\omega)\,\omega^4}\,T(\omega)\,d\omega$$

INCLUDE EMISSION SPECTRUM

$$\int_0^\infty \delta(\omega-\omega_o)\, d\omega \;=\; 1 \quad\longrightarrow\quad \int_0^\infty f_D(\omega)\, d\omega \;=\; 1$$

$$\frac{\gamma_{D\rightarrow A}}{\gamma_o} \;=\; \frac{9c^4}{8\pi R^6} \int_0^\infty \frac{f_D(\omega)\, \sigma_A(\omega)}{n^4(\omega)\, \omega^4}\, T(\omega)\, d\omega$$

Evaluate T(ω) :

$$\begin{aligned} T(\omega) \;=\; & (1-k^2R^2+k^4R^4)\,(\mathbf{n}_A\cdot\mathbf{n}_D)^2 \;+ \\ & (9+3k^2R^2+k^4R^4)\,(\mathbf{n}_R\cdot\mathbf{n}_D)^2(\mathbf{n}_R\cdot\mathbf{n}_A)^2 \;+ \\ & (-6+2k^2R^2-2k^4R^4)\,(\mathbf{n}_A\cdot\mathbf{n}_D)(\mathbf{n}_R\cdot\mathbf{n}_D)(\mathbf{n}_R\cdot\mathbf{n}_A) \end{aligned}$$

$$\langle T(\omega)\rangle \;=\; \frac{2}{3} \;+\; \frac{2}{9}k^2R^2 \;+\; \frac{2}{9}k^4R^4$$

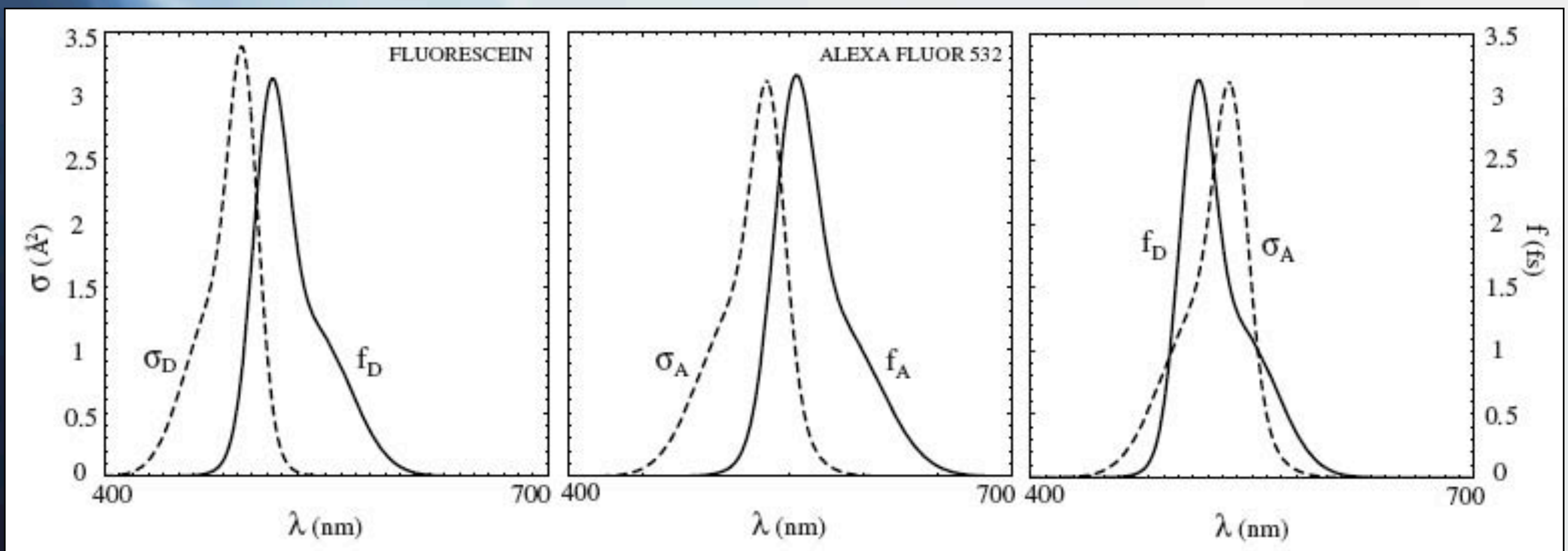
ONLY NEAR-FIELD TERMS

$$\frac{\gamma_{D\rightarrow A}}{\gamma_o} = \left[\frac{R_o}{R}\right]^6 , \qquad R_o^6 = \frac{9\,c^4\,\kappa^2}{8\pi}\int\limits_0^\infty \frac{f_D(\omega)\;\sigma_A(\omega)}{n^4(\omega)\,\omega^4}\,d\omega$$

$$\kappa^2 = [\mathbf{n}_A\cdot\mathbf{n}_D - 3\,(\mathbf{n}_R\cdot\mathbf{n}_D)(\mathbf{n}_R\cdot\mathbf{n}_A)]^2$$

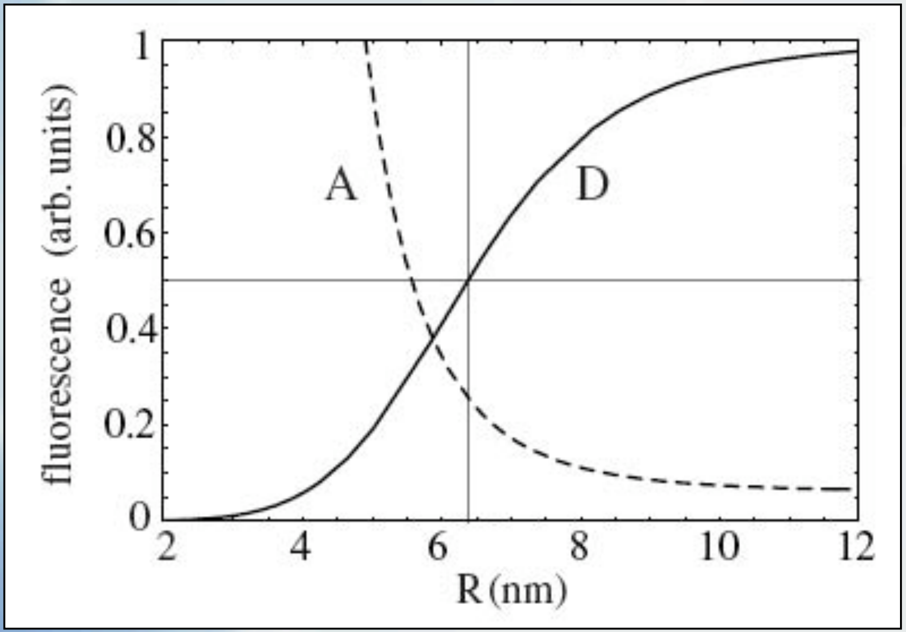
EXAMPLE:
Alexa Fluor 532 (A) and Fluorescein (D)

Fitting : $\sum_{n=1}^{N} A_n e^{-(\lambda-\lambda_n)^2/\Delta\lambda_n^2}$



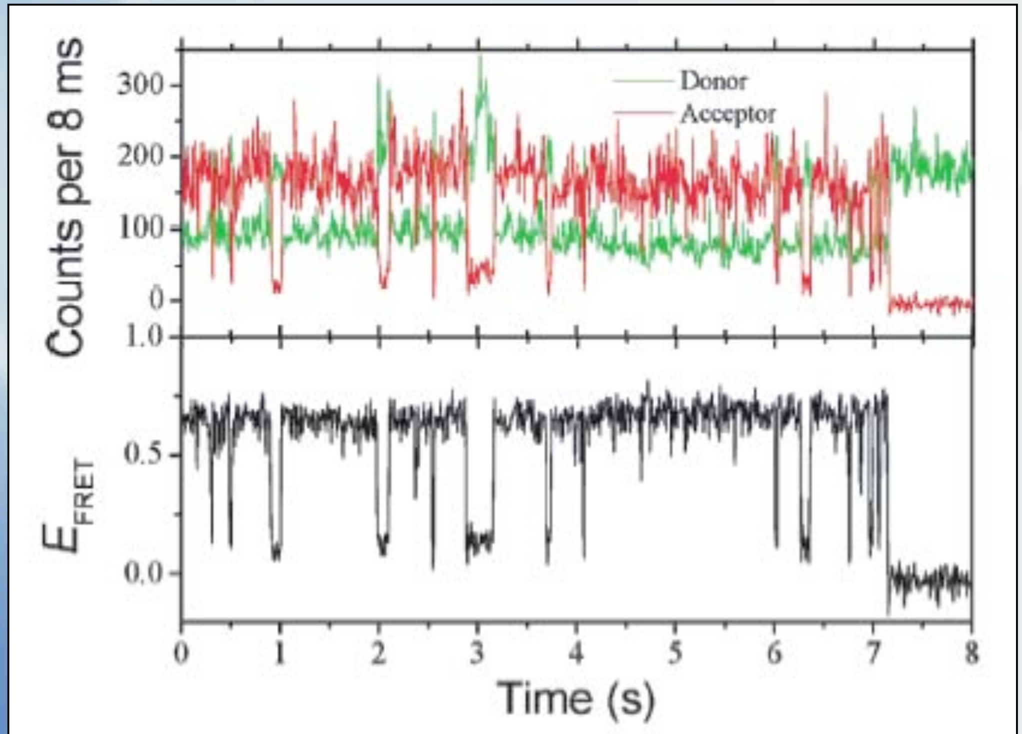
Water: R_o = 6.3nm ; Air: R_o = 7.6nm

DONOR / ACCEPTOR FLUORESCENCE



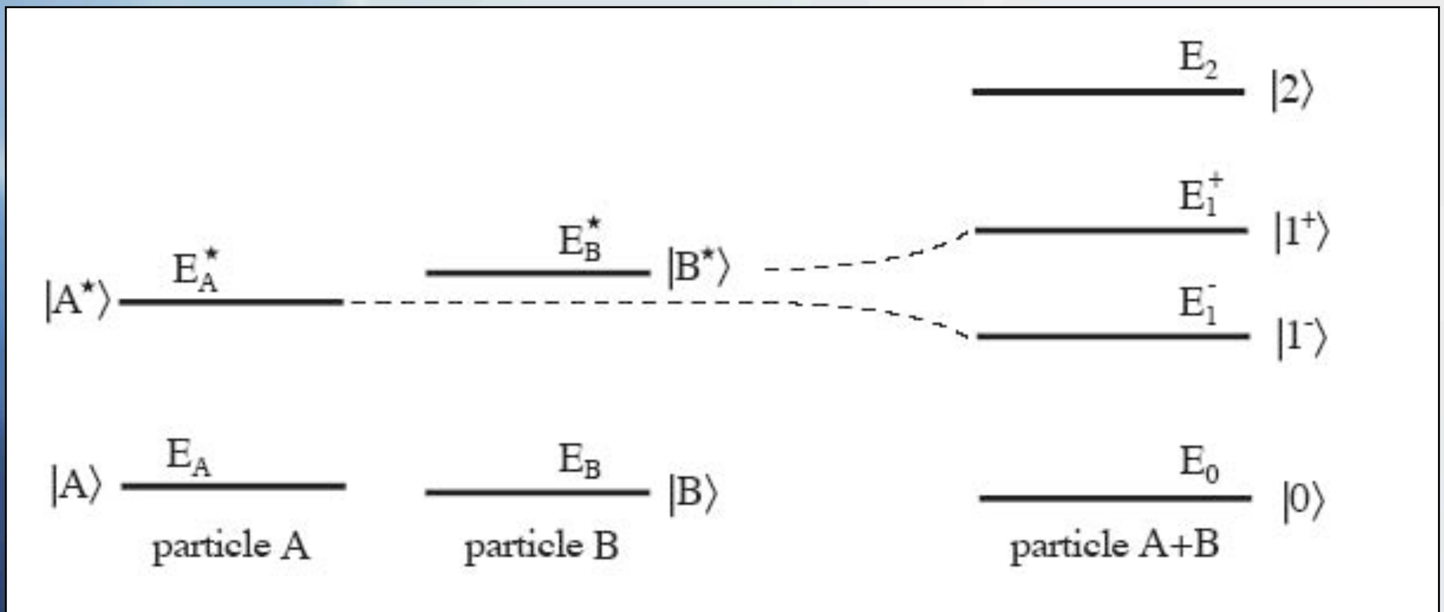
$$E = \frac{P_o}{P_o + P_{D\to A}} = \frac{1}{1 + (\gamma_o/\gamma_{D\to A})} = \frac{1}{1 + (R/R_o)^6}$$

EXAMPLE: DNA HOLIDAY JUNCTION



Taekjip Ha (Urbana-Champaign)

STRONG COUPLING REGIME



$$|1^+\rangle = \cos\alpha\,|A^\star B\rangle + \sin\alpha\,|AB^\star\rangle$$
$$|1^-\rangle = \sin\alpha\,|A^\star B\rangle - \cos\alpha\,|AB^\star\rangle$$

SUMMARY

FRET IS A POWERFUL TECHNIQUE TO MEASURE NANOSCALE DISTANCES

EFFECT CAN BE UNDERSTOOD BASED ON ANTENNA THEORY

- Gives correct Result for Near-field, Intermediate Field, and Farfield
- Strong Coupling Regime requires QM