COMSOL SIMULATION OF CHIRAL MOLECULE INTERACTION WITH CHIRAL STRUCTURES.

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COMSOL CONFERENCE
ROTTERDAM 2013

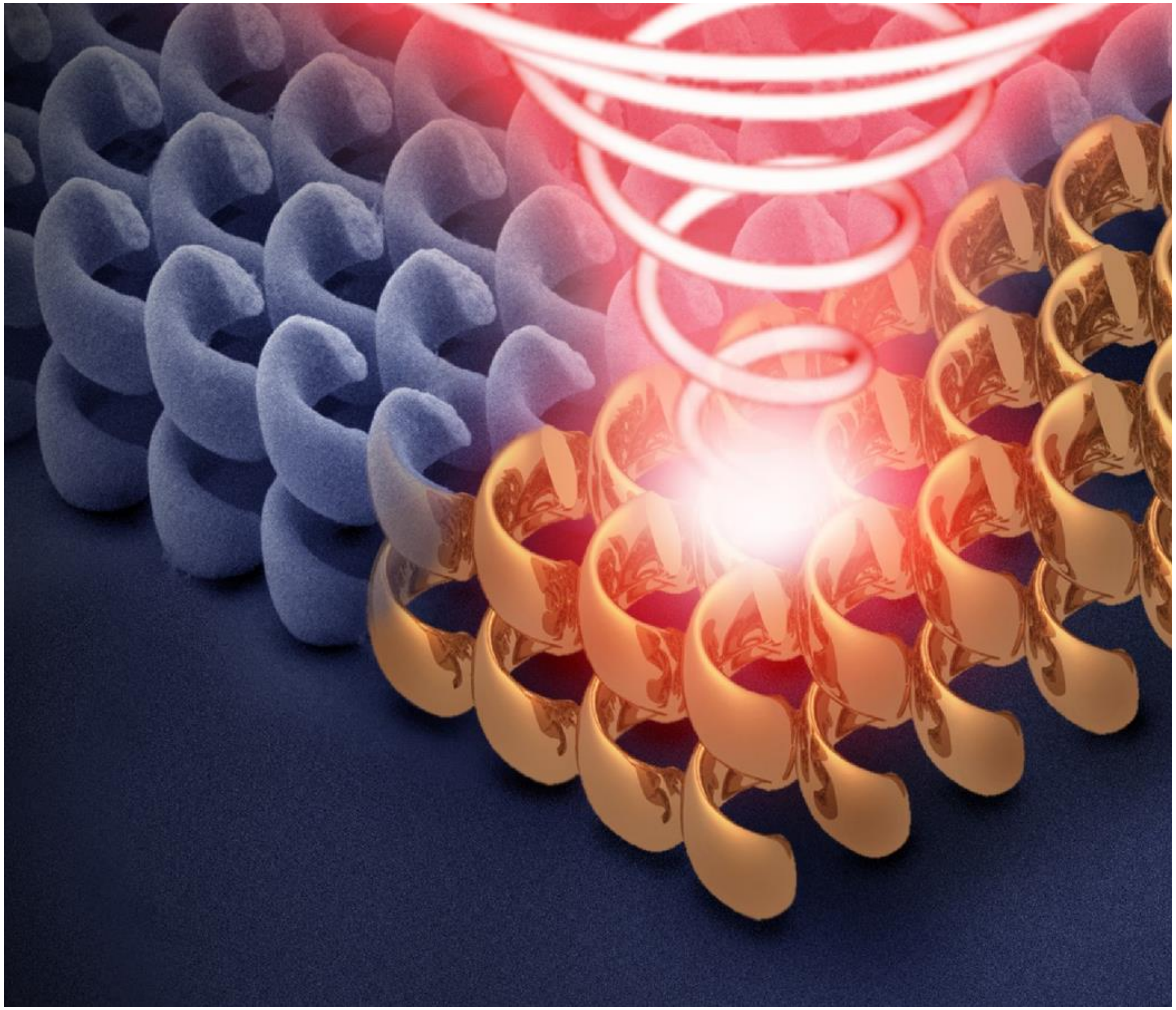
CHIRALITY AND OPTICAL ACTIVITY

Chirality is the property of system do not coincide with their mirror reflection.

CHIRALITY AND OPTICAL ACTIVITY

$$\mathbf{D} = \varepsilon\left(\mathbf{E} + \eta \mathrm{rot}\mathbf{E}\right)$$

$$\mathbf{B} = \mu\left(\mathbf{H} + \eta \mathrm{rot}\mathbf{H}\right)$$



Gold Helix Metamaterial

(Gansel et al., Science, 2009)

PURCELL EFFECT (1946)

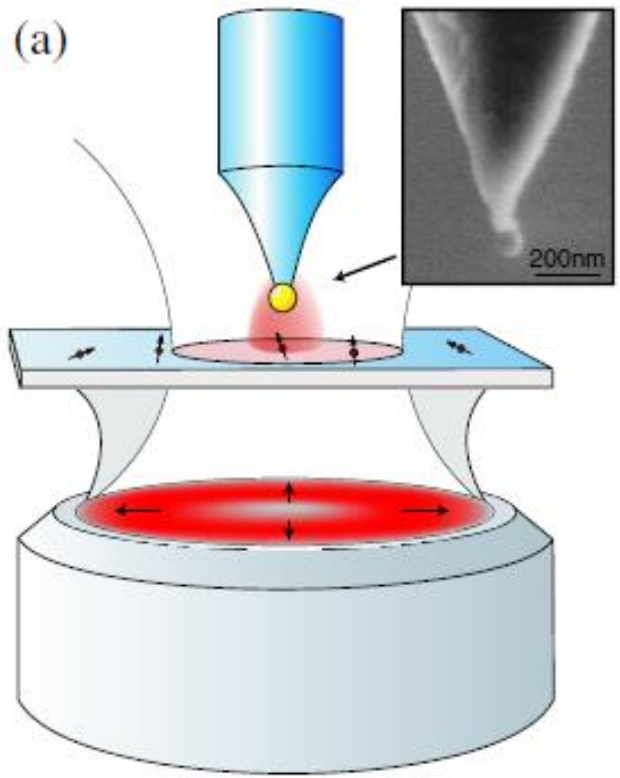
Decay rate depend significantly on nano enviroment

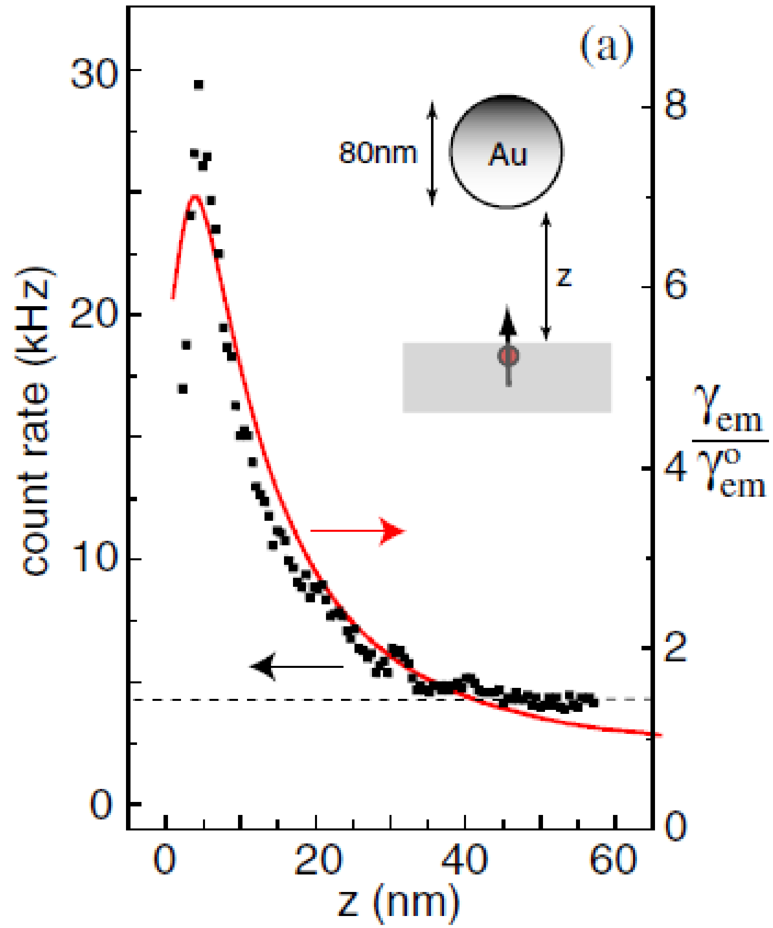
B10. Spontaneous Emission Probabilities at Radio Frequencies. E. M. PURCELL, *Harvard University.*—For nuclear magnetic moment transitions at radio frequencies the probability of spontaneous emission, computed from

$$A_\nu = (8\pi\nu^2/c^3)h\nu(8\pi^3\mu^2/3h^2) \text{ sec.}^{-1},$$

is so small that this process is not effective in bringing a

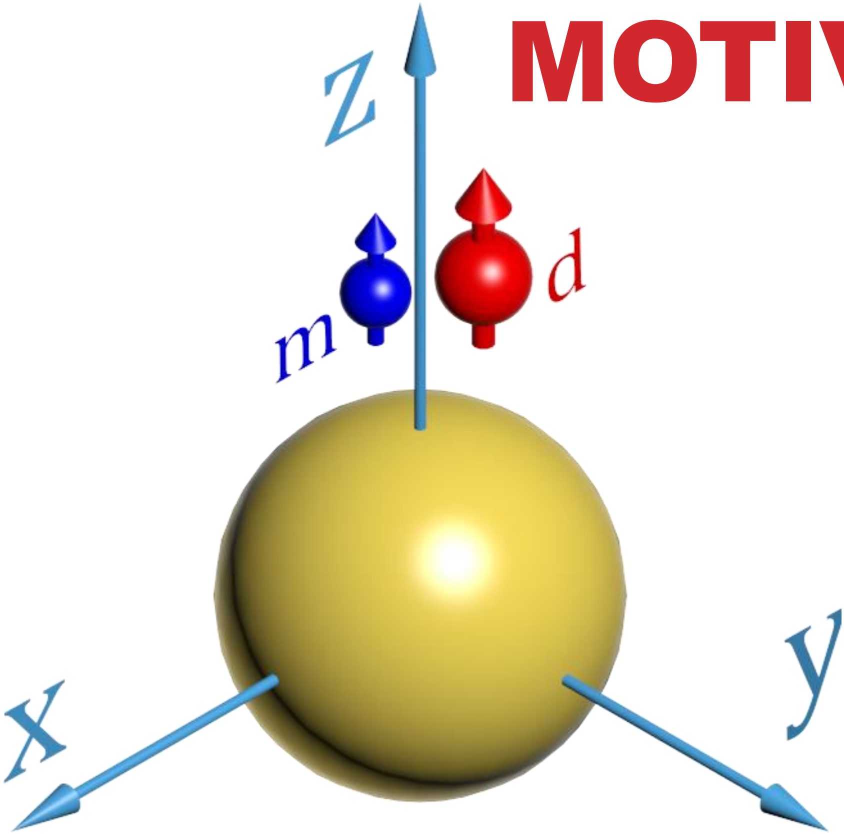
ENHANCEMENT AND QUENCHING OF SINGLE-MOLECULE FLUORESCENCE





ANGER, P., BHARADWAJ, P., & NOVOTNY, L. (2006). ENHANCEMENT AND QUENCHING OF SINGLE-MOLECULE FLUORESCENCE. *PHYSICAL REVIEW LETTERS*, *96*(11), 113002. DOI:10.1103/PHYSREVLETT.96.113002

MOTIVATION



$$\gamma_{eg}^{A,-1}=\frac{k_0}{2\hbar r_0^2}\sum_{n=1}^{\infty}\frac{2n+1}{1+\left|O_n\right|^2}\Big|\left(d_{0x}-id_{0y}\right)\left(\psi_n'\left(k_0r_0\right)+T_n^A\zeta_n^{(1)\prime}\left(k_0r_0\right)\right)$$

$$-O_n\left(d_{0y}+id_{0x}\right)\left(\psi_n\left(k_0r_0\right)+L_n^A\zeta_n^{(1)}\left(k_0r_0\right)\right)$$

$$+O_n\left(m_{0x}-im_{0y}\right)\left(\psi_n'\left(k_0r_0\right)+L_n^A\zeta_n^{(1)\prime}\left(k_0r_0\right)\right)$$

$$-\left(m_{0y}+im_{0x}\right)\left(\psi_n\left(k_0r_0\right)+T_n^A\zeta_n^{(1)}\left(k_0r_0\right)\right)\Big|^2,$$

$$\gamma_{eg}^{A,1}=\frac{k_0}{2\hbar r_0^2}\sum_{n=1}^{\infty}\frac{2n+1}{1+\left|O_n\right|^2}\Big|O_n\left(d_{0y}-id_{0x}\right)\left(\psi_n\left(k_0r_0\right)+L_n^A\zeta_n^{(1)}\left(k_0r_0\right)\right)$$

$$-\left(d_{0x}+id_{0y}\right)\left(\psi_n'\left(k_0r_0\right)+T_n^A\zeta_n^{(1)\prime}\left(k_0r_0\right)\right)$$

$$+\left(m_{0y}-im_{0x}\right)\left(\psi_n\left(k_0r_0\right)+T_n^A\zeta_n^{(1)}\left(k_0r_0\right)\right)$$

$$-O_n\left(m_{0x}+im_{0y}\right)\left(\psi_n'\left(k_0r_0\right)+L_n^A\zeta_n^{(1)\prime}\left(k_0r_0\right)\right)\Big|^2,$$

$$\gamma_{eg}=\gamma_{eg}^{A}+\gamma_{eg}^{B}$$

$$\gamma_{eg}^{A}=\gamma_{eg}^{A,-1}+\gamma_{eg}^{A,1}+\gamma_{eg}^{A,0}$$

$$\gamma_{eg}^{A,0}=\frac{2}{\hbar k_0 r_0^4}\sum_{n=1}^{\infty}\frac{(2n+1)n(n+1)}{1+\left|O_n\right|^2}\Big|d_{0z}\left(\psi_n\left(k_0r_0\right)+T_n^A\zeta_n^{(1)}\left(k_0r_0\right)\right)$$

$$+O_nm_{0z}\left(\psi_n\left(k_0r_0\right)+L_n^A\zeta_n^{(1)}\left(k_0r_0\right)\right)\Big|^2.$$

$$T_n^A=\frac{1}{4}\left(\alpha_n-\gamma_n+\sqrt{\left(\alpha_n+\gamma_n\right)^2-4\beta_n^2}-2\right),\quad L_n^A=\frac{1}{4}\left(\gamma_n-\alpha_n-\sqrt{\left(\alpha_n+\gamma_n\right)^2-4\beta_n^2}-2\right),$$

$$T_n^B=\frac{1}{4}\left(\alpha_n-\gamma_n-\sqrt{\left(\alpha_n+\gamma_n\right)^2-4\beta_n^2}-2\right),\quad L_n^B=\frac{1}{4}\left(\gamma_n-\alpha_n+\sqrt{\left(\alpha_n+\gamma_n\right)^2-4\beta_n^2}-2\right).$$

WAVE EQUATIONS

Normal media

$$rot\left(\frac{1}{\mu}rot\,\mathbf{E}\right)-k_0^2\varepsilon\mathbf{E}=0$$

Chiral media

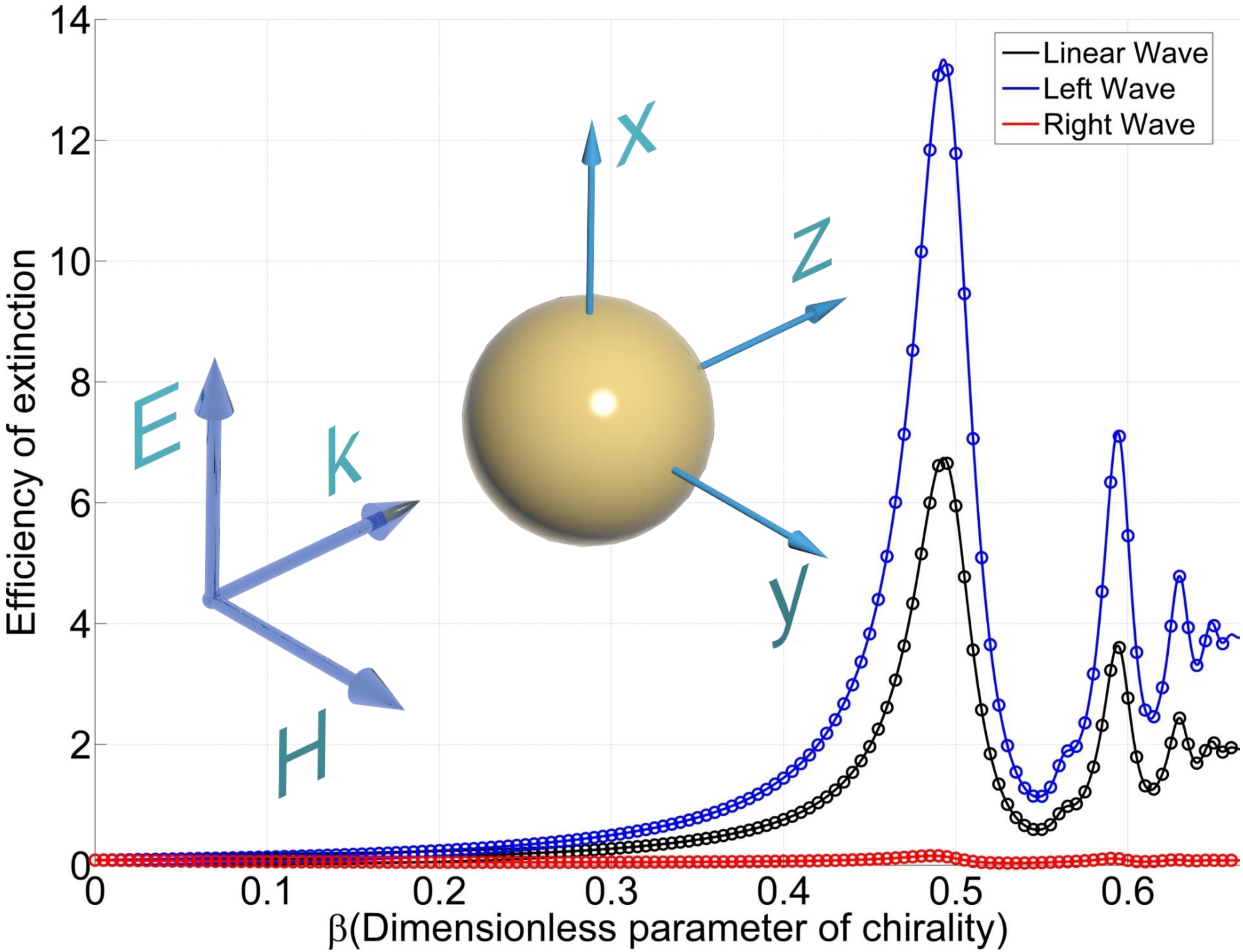
$$rot\left(\frac{1}{\mu}rot\,\mathbf{E}\left(1-k_0^2\eta^2\varepsilon\mu\right)\right)$$

$$-k_0^2\,rot\left(\varepsilon\eta\mathbf{E}\right)-k_0^2\varepsilon\eta rot\,\mathbf{E}-k_0^2\varepsilon\mathbf{E}=0$$

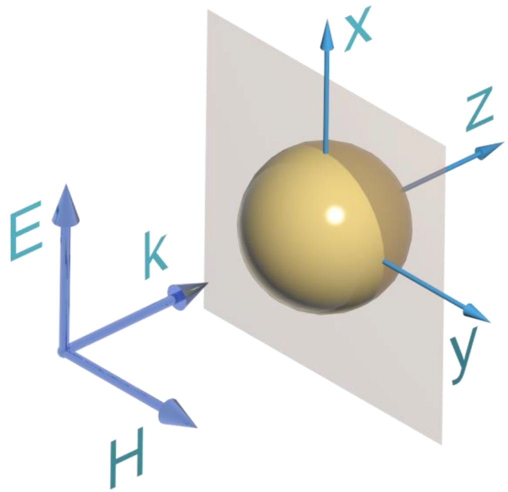
$$\mathbf{H}=\frac{1}{ik_0}\left[\frac{1}{\mu}rot\,\mathbf{E}\left(1-k_0^2\eta^2\varepsilon\mu\right)-k_0^2\eta\varepsilon\mathbf{E}\right]$$

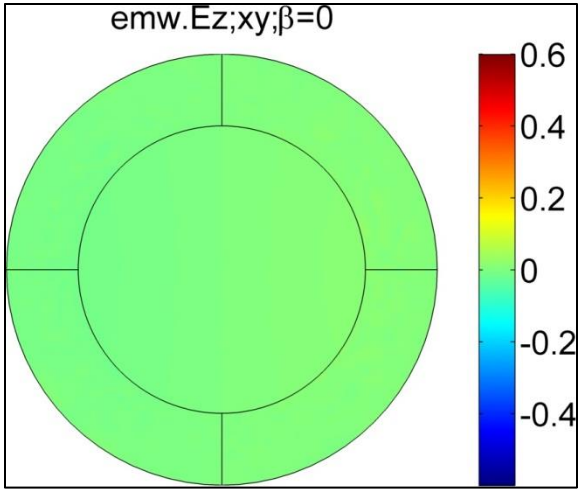
Changing wave equation and adding boundary current

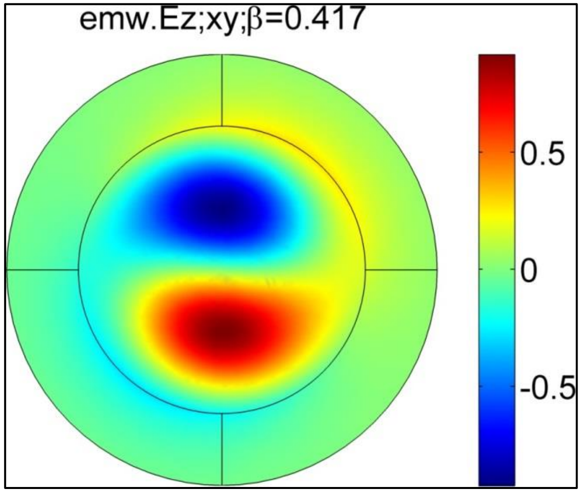
CHIRAL DIELECTRIC SPHERE AND PLANE WAVE

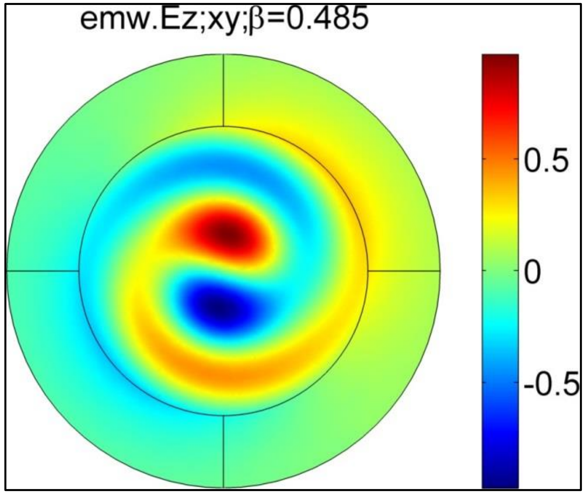


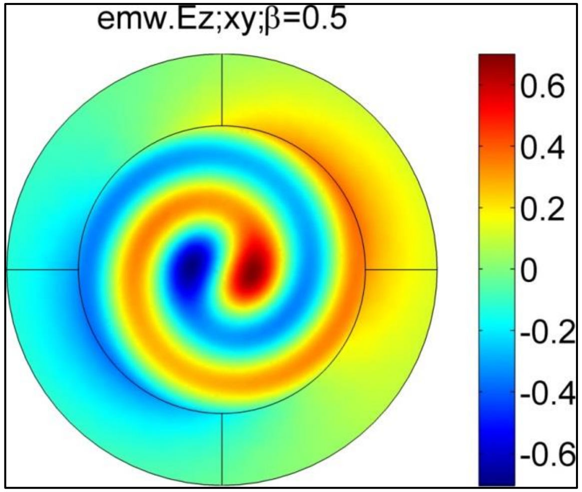
TWISTING OF FIELD

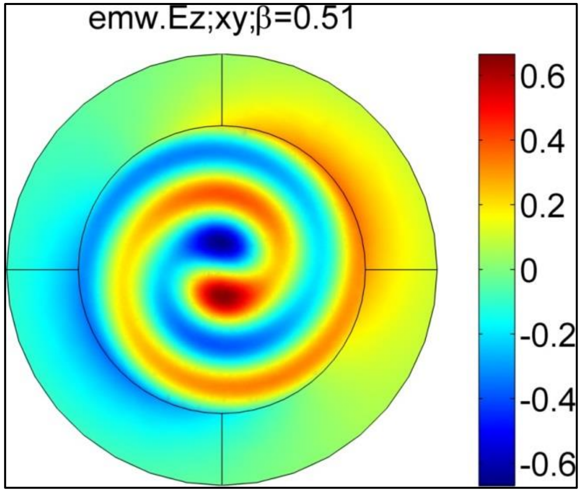




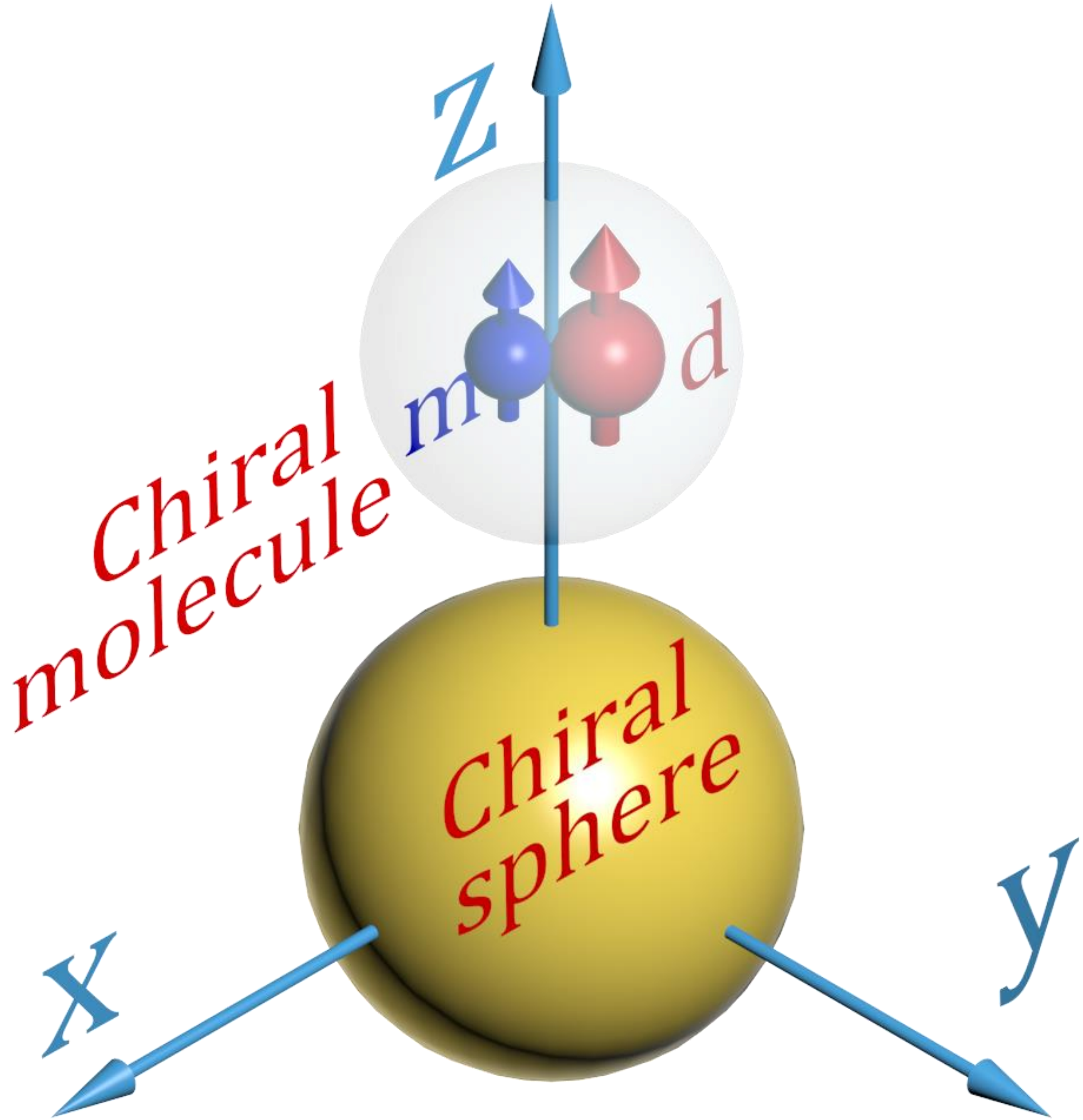


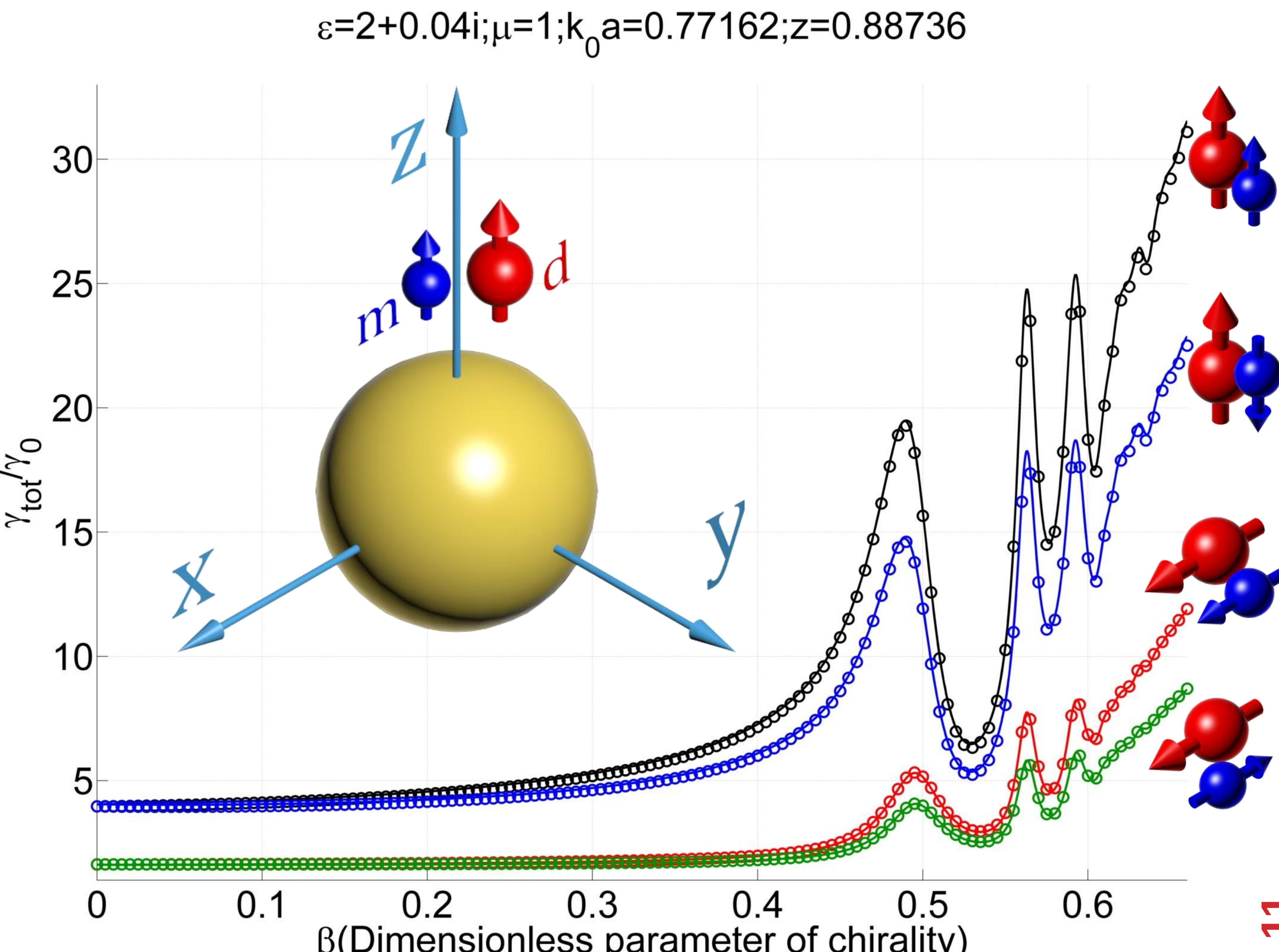






GEOMETRY OF THE PROBLEM OF RADIATION OF CHIRAL MOLECULE IN THE VICINITY OF CHIRAL SPHERE.




ε=2+0.04i;μ=1;k_0a=0.77162;z=0.88736
γ_{tot}/γ_0
β(Dimensionless parameter of chirality)
z
x
y
m
d
0
0.1
0.2
0.3
0.4
0.5
0.6
5
10
15
20
25
30

CONCLUSIONS

- RF module was modified in order to work with chiral structures.
- Obtained numerical results verified complicated analytical results.
- Moreover it gives the powerful tool to study interaction of light with chiral structures.

ACKNOWLEDGMENTS

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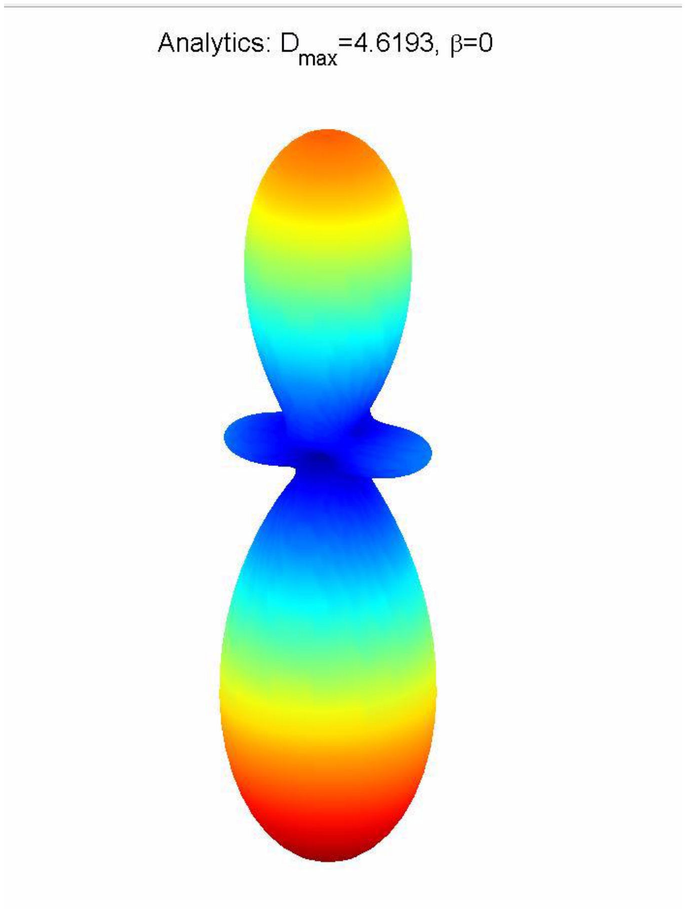
- **the Russian Quantum Center and Skolkovo foundation**

RADIATION PATTERN OF DIPOLE NEAR SI SPHERE



$$l = 455nm$$

$$r = 90nm$$

$$e = 21.28 + 1.209i$$

$$m = 1$$

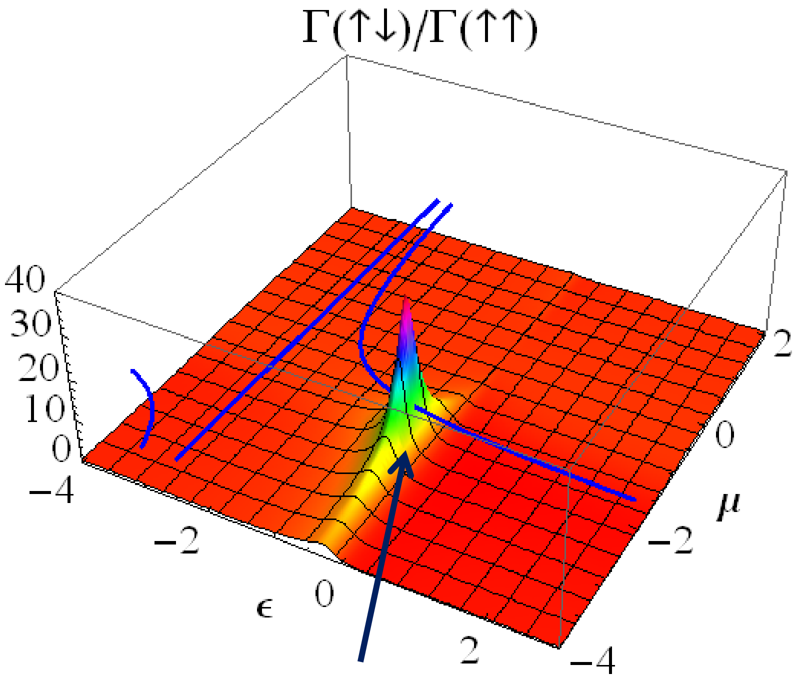
$$\mathbf{d} = (1, 0, 0)$$

$$\mathbf{r}_d = (0, 0, r + 2nm)$$

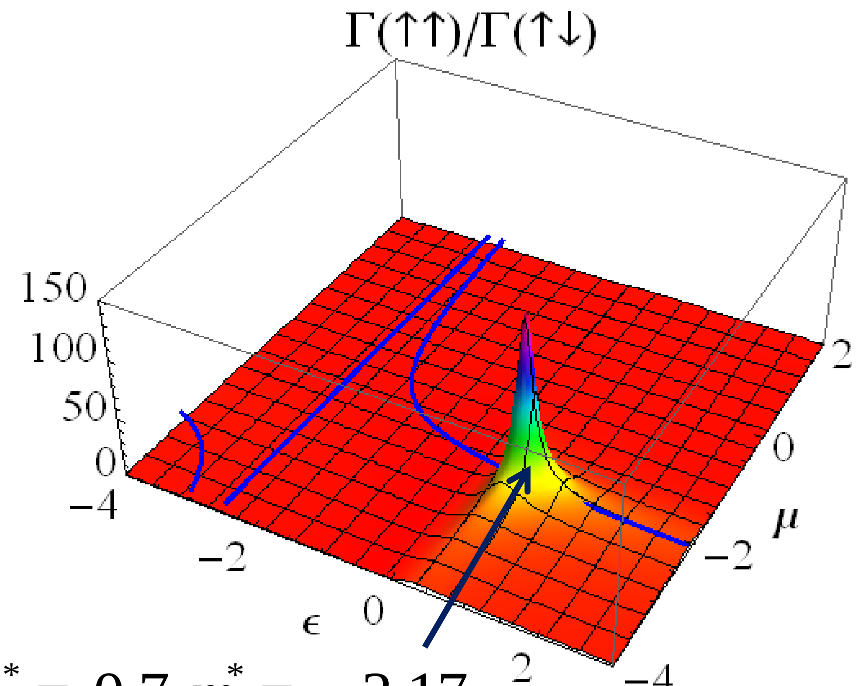
$$b = 0 - 0.3$$

EFFECTIVE RADIATIVE DECAY RATE OF A CHIRAL MOLECULE PLACED IN THE VICINITY OF A CHIRAL SPHERE (KLIMOV GUZATOV DUCLOY EPL 2012).

$$c = 0.2, m_{0z} / d_{0z} = 0.2; e' = 0.1, k_0 a = 0.1$$



$e^* = -0.667, m^* = -1.85$



$e^* = 0.7, m^* = -2.17$

This example shows that DNG or MNG chiral nanoparticles allow discrimination of radiation of chiral molecule indeed. It is very important that negative refractive index or negative magnetic permittivity are necessary condition for this effect.

TOTAL DECAY RATE

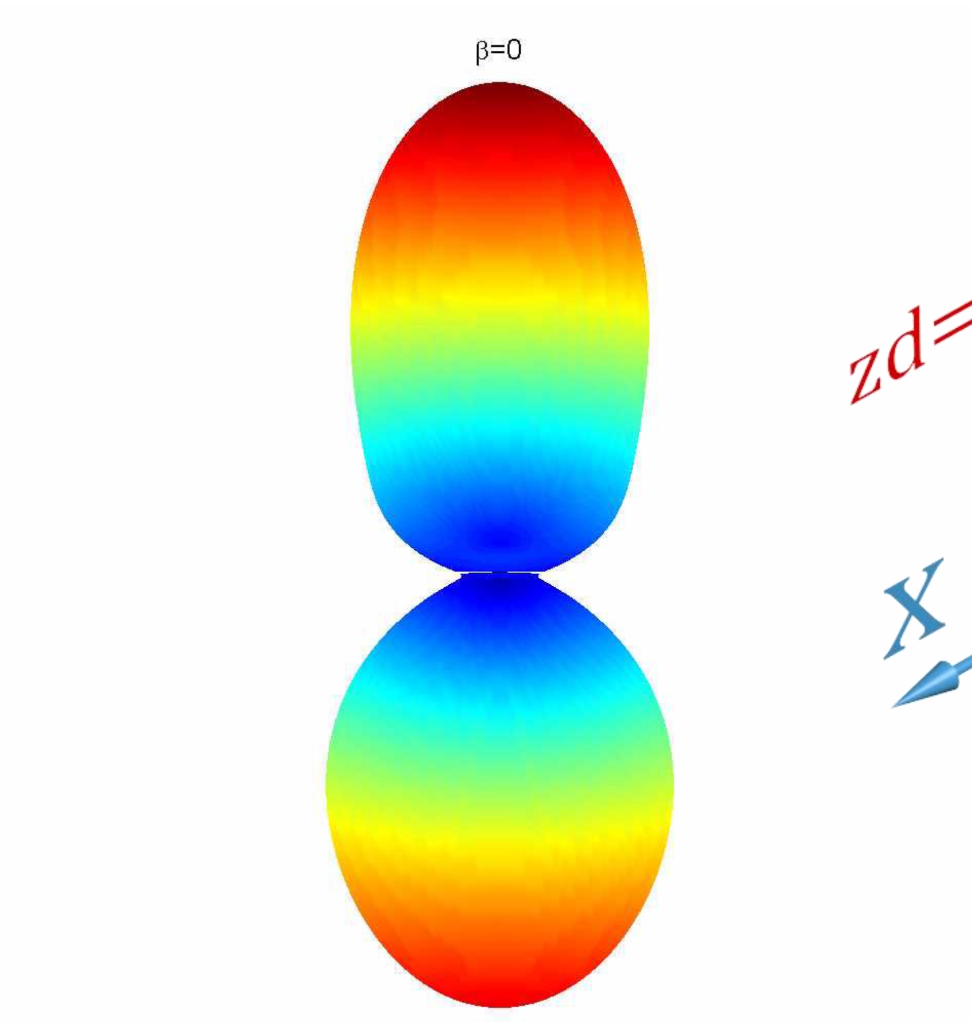
The rate of spontaneous emission is strongly dependent on nano-environment. (Purcell effect)

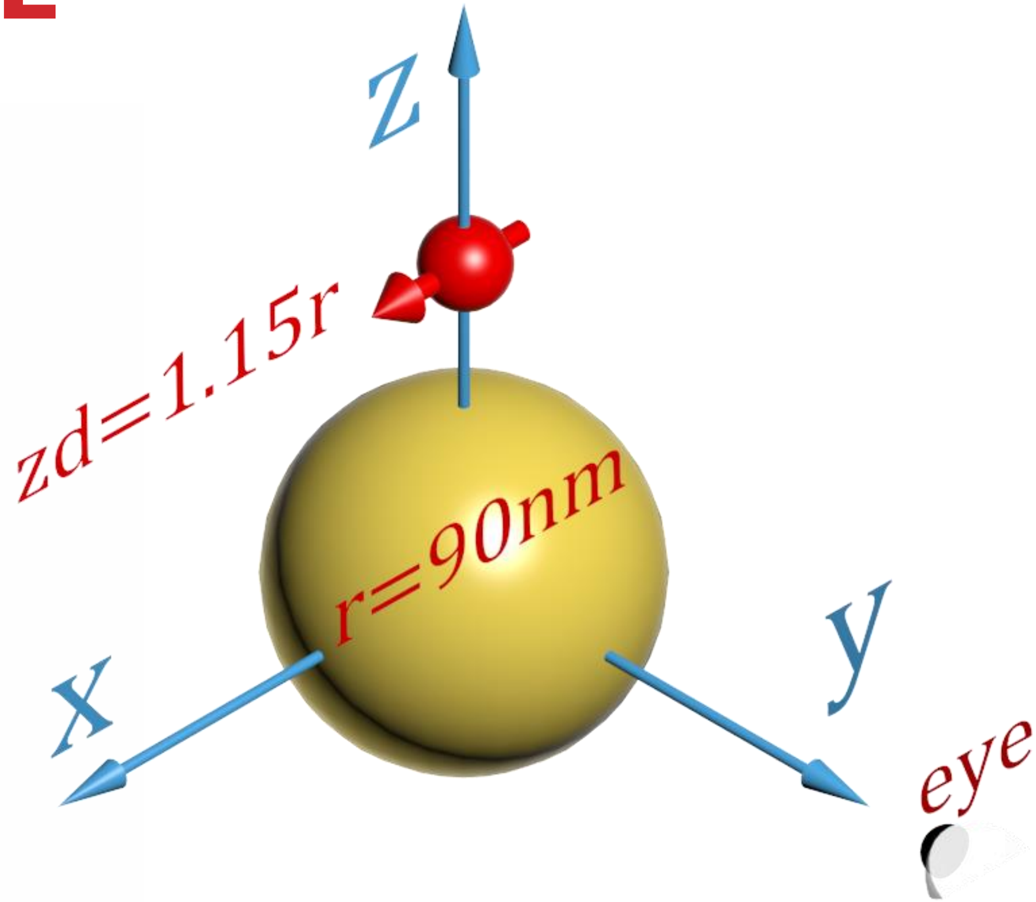
The total decay rate of the spontaneous emission can be found as the ratio of the work done by the molecule with particle over field to the work done by the molecule in free space:

$$\frac{\gamma_{tot}}{\gamma_0} = 1 + \frac{3}{2}\,\mathrm{Im}\left\{\frac{\mathbf{d}_0^* \cdot \mathbf{E}^{refl}(\mathbf{r}_0) + i\mathbf{m}_0^* \cdot \mathbf{H}^{refl}(\mathbf{r}_0)}{k_0^3\left(|\mathbf{d}_0|^2 + |\mathbf{m}_0|^2\right)}\right\}$$

Klimov, Guzatov, New Journal of Physics 14 (2012) 123009

RADIATION PATTERN OF DIPOLE NEAR SI SPHERE





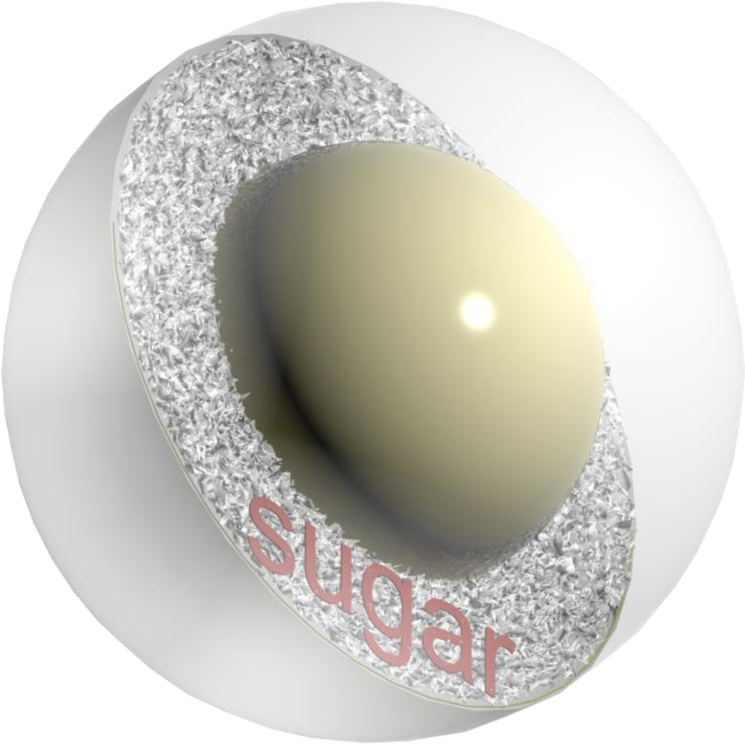
$l = 455nm$

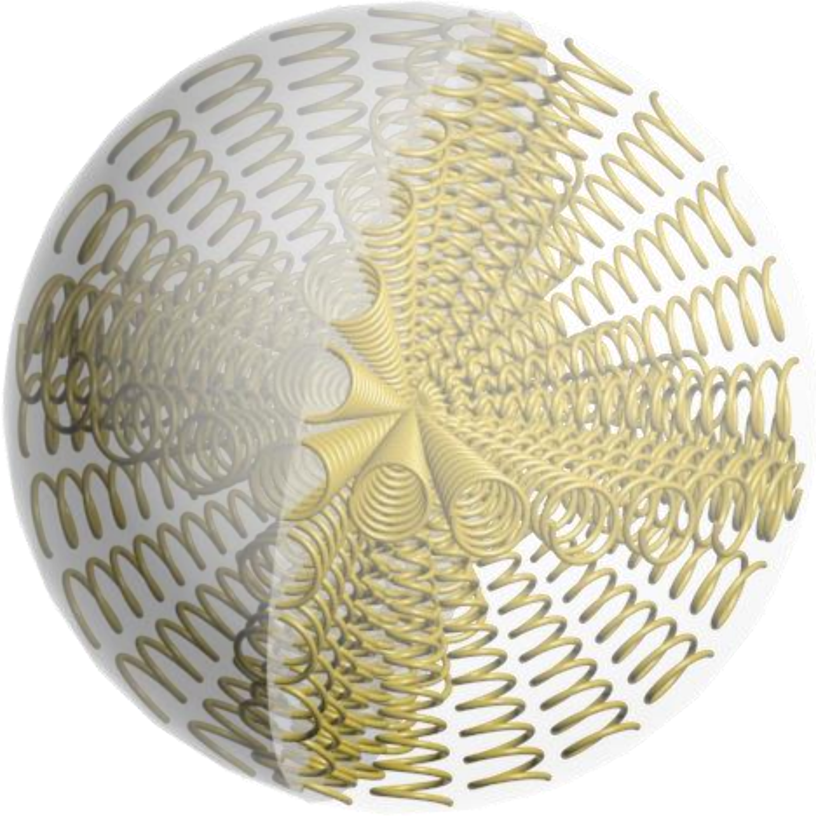
$e = 21.28 + 1.209i$

$m = 1$

$b = 0 - 0.25$

THE SIMPLEST MODEL OF CHIRAL SPHERE





Dimensionless parameter of chirality: $\beta = k_0 \chi$

FUNDAMENTAL MODES IN CHIRAL MEDIA

$$\mathbf{D} = \varepsilon\left(\mathbf{E} + \chi \mathrm{rot}\mathbf{E}\right),\ \mathbf{B} = \mu\left(\mathbf{H} + \chi \mathrm{rot}\mathbf{H}\right)$$

$$\mathbf{E} = \mathbf{Q}_L + b\mathbf{Q}_R,\ \ \mathbf{H} = c\mathbf{Q}_L + \mathbf{Q}_R, b = -i\mu/\sqrt{\varepsilon\mu}; d = -i\sqrt{\varepsilon\mu}/\mu$$

$$\mathrm{rot}\mathbf{Q}_L = +k_L\mathbf{Q}_L,\quad \mathrm{div}\mathbf{Q}_L = 0,\ \mathrm{rot}\mathbf{Q}_R = -k_R\mathbf{Q}_R,\quad \mathrm{div}\mathbf{Q}_R = 0$$

$$k_L = \frac{k_0\sqrt{\varepsilon\mu}}{1-\chi\sqrt{\varepsilon\mu}},\quad k_R = \frac{k_0\sqrt{\varepsilon\mu}}{1+\chi\sqrt{\varepsilon\mu}}$$

$$\mathbf{Q}_L = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} A_{mn}\left(\mathbf{N}\boldsymbol{\psi}_{mn}^{(L)} + \mathbf{M}\boldsymbol{\psi}_{mn}^{(L)}\right),$$

$$\mathbf{Q}_R = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} B_{mn}\left(\mathbf{N}\boldsymbol{\psi}_{mn}^{(R)} - \mathbf{M}\boldsymbol{\psi}_{mn}^{(R)}\right)$$

$\mathbf{N}\boldsymbol{\psi}_{mn}^{(L)}, \mathbf{M}\boldsymbol{\psi}_{mn}^{(L)}, \mathbf{N}\boldsymbol{\psi}_{mn}^{(R)}, \mathbf{M}\boldsymbol{\psi}_{mn}^{(R)}$ - Vector spherical harmonics

DECAY RATE OF ATOM

CLASSICAL ELECTRODYNAMICS

$$\mathbf{j}(\mathbf{r},t) = i\omega\mathbf{d}\,\delta(\mathbf{r}-\mathbf{r}_0)$$

$$\frac{P}{P_0} = 1 + \frac{6\pi\varepsilon_0}{|\mathbf{d}|^2}\frac{1}{k^3}\,\mathrm{Im}\left[\mathbf{d}^*\mathbf{E}_s(\mathbf{r}_0)\right]$$

QUANTUM ELECTODYNAMICS

$$\gamma = \frac{2\pi}{\hbar}\sum_f \left|\langle f|\hat{V}|i\rangle\right|\delta(\omega_i - \omega_f)$$

$$\gamma = \frac{2\omega_0}{3\hbar\varepsilon_0}|\mathbf{d}|^2\,\rho_\mu(\mathbf{r}_0,\omega_0)$$

$$\rho_\mu(\mathbf{r}_0,\omega_0) = \frac{6\omega_0}{\pi c^2}\left\{\mathbf{n}_d\,\mathrm{Im}\left[\overset{\leftrightarrow}{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_0)\mathbf{n}_d\right]\right\}$$

$$\frac{\gamma}{\gamma_0} = 1 + \frac{6\pi\varepsilon_0}{|\mathbf{d}|^2}\frac{1}{k^3}\,\mathrm{Im}[\mathbf{d}^*\mathbf{E}_s(\mathbf{r}_0)]$$