COMSOL SIMULATION OF CHIRAL MOLECULE INTERACTION WITH CHIRAL STRUCTURES.

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Chirality is the property of a system that do not coincide with their mirror reflection.
CHIRALITY AND OPTICAL ACTIVITY

\[ \mathbf{D} = \varepsilon (\mathbf{E} + \eta \text{rotE}) \]

\[ \mathbf{B} = \mu (\mathbf{H} + \eta \text{rotH}) \]

Gold Helix
Metamaterial

(Gansel et al., Science, 2009)
Decay rate depend significantly on nano envirnoment

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

\[ A_r = \frac{8\pi v^2}{c^3} \hbar v \left( \frac{8\pi^3 \mu^2}{3\hbar^3} \right) \text{ sec}^{-1}, \]

is so small that this process is not effective in bringing a
ENHANCEMENT AND QUENCHING OF SINGLE-MOLECULE FLUORESCENCE

**MOTIVATION**

\[ \gamma_{eg}^{A,-1} = \frac{k_n}{2\hbar r_0^2} \sum_{n=1}^{\infty} \frac{2n+1}{1+|O_n|^2} \left| (d_{0x} - id_{0y}) \left( \psi_n'(k_0 r_0) + T_n^{A} \zeta_n^{(1)'}(k_0 r_0) \right) \right| \]
\[ - O_n \left( d_{0y} + id_{0x} \right) \left( \psi_n(k_0 r_0) + L_n^{A} \zeta_n^{(1)}(k_0 r_0) \right) \]
\[ + O_n \left( m_{0x} - im_{0y} \right) \left( \psi_n'(k_0 r_0) + L_n^{A} \zeta_n^{(1)'}(k_0 r_0) \right) \]
\[ - \left( m_{0y} + im_{0x} \right) \left( \psi_n(k_0 r_0) + T_n^{A} \zeta_n^{(1)}(k_0 r_0) \right) \right|^2, \]

\[ \gamma_{eg}^{A,1} = \frac{k_0}{2\hbar r_0^2} \sum_{n=1}^{\infty} \frac{2n+1}{1+|O_n|^2} \left| O_n \left( d_{0y} - id_{0x} \right) \left( \psi_n(k_0 r_0) + L_n^{A} \zeta_n^{(1)}(k_0 r_0) \right) \right| \]
\[ - \left( d_{0x} + id_{0y} \right) \left( \psi_n'(k_0 r_0) + T_n^{A} \zeta_n^{(1)'}(k_0 r_0) \right) \]
\[ + \left( m_{0y} - im_{0x} \right) \left( \psi_n(k_0 r_0) + T_n^{A} \zeta_n^{(1)}(k_0 r_0) \right) \]
\[ - O_n \left( m_{0x} + im_{0y} \right) \left( \psi_n'(k_0 r_0) + L_n^{A} \zeta_n^{(1)'}(k_0 r_0) \right) \right|^2, \]

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

\[ T_n^{A} = \frac{1}{4} \left( \alpha_n - \gamma_n + \sqrt{(\alpha_n + \gamma_n)^2 - 4\beta_n^2} - 2 \right), \quad L_n^{A} = \frac{1}{4} \left( \gamma_n - \alpha_n - \sqrt{(\alpha_n + \gamma_n)^2 - 4\beta_n^2} - 2 \right), \]
\[ T_n^{B} = \frac{1}{4} \left( \alpha_n - \gamma_n - \sqrt{(\alpha_n + \gamma_n)^2 - 4\beta_n^2} - 2 \right), \quad L_n^{B} = \frac{1}{4} \left( \gamma_n - \alpha_n + \sqrt{(\alpha_n + \gamma_n)^2 - 4\beta_n^2} - 2 \right). \]
Normal media
\[ \text{rot} \left( \frac{1}{\mu} \text{rot} \mathbf{E} \right) - k_0^2 \varepsilon \mathbf{E} = 0 \]

Chiral media
\[ \text{rot} \left( \frac{1}{\mu} \text{rot} \mathbf{E} \left( 1 - k_0^2 \eta^2 \varepsilon \mu \right) \right) - k_0^2 \text{rot} \left( \varepsilon \eta \mathbf{E} \right) - k_0^2 \varepsilon \eta \text{rot} \mathbf{E} - k_0^2 \varepsilon \mathbf{E} = 0 \]

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

Changing wave equation and adding boundary current
CHIRAL DIELECTRIC SPHERE AND PLANE WAVE

Efficiency of extinction

$\beta$ (Dimensionless parameter of chirality)
TWISTING OF FIELD

emw.Ez;xy;β=0

emw.Ez;xy;β=0.417

emw.Ez;xy;β=0.485

emw.Ez;xy;β=0.5

emw.Ez;xy;β=0.51
GEOMETRY OF THE PROBLEM OF RADIATION OF CHIRAL MOLECULE IN THE VICINITY OF CHIRAL SPHERE.
$\varepsilon=2+0.04i; \mu=1; k_0a=0.77162; z=0.88736$
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.
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RADIATION PATTERN OF DIPOLE NEAR SI SPHERE

\[ l = 455nm \]
\[ r = 90nm \]
\[ e = 21.28 + 1.209i \]
\[ m = 1 \]
\[ d = (1, 0, 0) \]
\[ \mathbf{r}_d = (0, 0, r + 2nm) \]
\[ b = 0 - 0.3 \]
EFFECTIVE RADIATIVE DECAY RATE OF A CHIRAL MOLECULE PLACED IN THE VICINITY OF A CHIRAL SPHERE (KLIMOV GUZATOV DUCLOY EPL 2012).

\[ c = 0.2, m_{0z} / d_{0z} = 0.2; e^\# = 0.1, k_0 a = 0.1 \]

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

RADIATION PATTERN OF DIPOLE NEAR SI SPHERE

\[ \beta = 0 \]

\[ zd = 1.15r \]

\[ r = 90\text{nm} \]

\[ l = 455\text{nm} \]

\[ e = 21.28 + 1.209i \]

\[ m = 1 \]

\[ b = 0 - 0.25 \]
THE SIMPLEST MODEL OF CHIRAL SPHERE

Dimensionless parameter of chirality: $\beta = k_0 \chi$
FUNDAMENTAL MODES IN CHIRAL MEDIA

\[
D = \varepsilon (E + \kappa \text{rot}E), \quad B = \mu (H + \kappa \text{rot}H)
\]

\[
E = Q_L + bQ_R, \quad H = cQ_L + Q_R, b = -i\mu / \sqrt{\varepsilon \mu}; d = -i\sqrt{\varepsilon \mu} / \mu
\]

\[
\text{rot}Q_L = +k_L Q_L, \quad \text{div}Q_L = 0, \quad \text{rot}Q_R = -k_R Q_R, \quad \text{div}Q_R = 0
\]

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

\[
Q_L = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} A_{mn} \left( N_{\psi_{mn}}^{(L)} + M_{\psi_{mn}}^{(L)} \right),
\]

\[
Q_R = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} B_{mn} \left( N_{\psi_{mn}}^{(R)} - M_{\psi_{mn}}^{(R)} \right)
\]

\[
N_{\psi_{mn}}^{(L)}, M_{\psi_{mn}}^{(L)}, N_{\psi_{mn}}^{(R)}, M_{\psi_{mn}}^{(R)} \quad - \text{Vector spherical harmonics}
\]


DECAY RATE OF ATOM

CLASSICAL ELECTRODYNAMICS

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

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

QUANTUM ELECTRODYNAMICS

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

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

\[
\rho_{\mu}(\mathbf{r}_0, \omega_0) = \frac{6\omega_0}{\pi c^2} \left\{ n_d \text{Im}\left[ \mathcal{G}(\mathbf{r}_0, \mathbf{r}_0, \omega_0) \mathbf{n}_d \right] \right\}
\]

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