2013 Ghana IGERT Presentation

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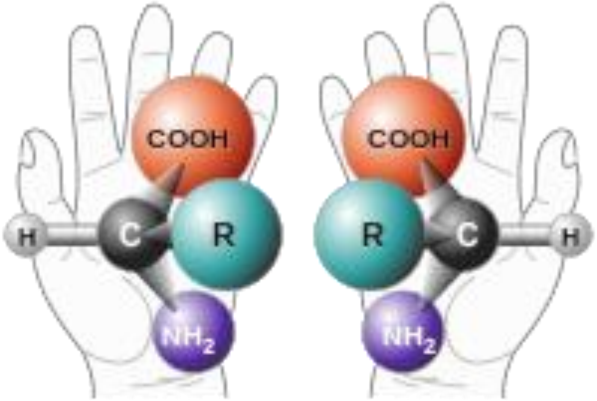
Part I: Background

Optical Activity and Chirality

Optical Activity

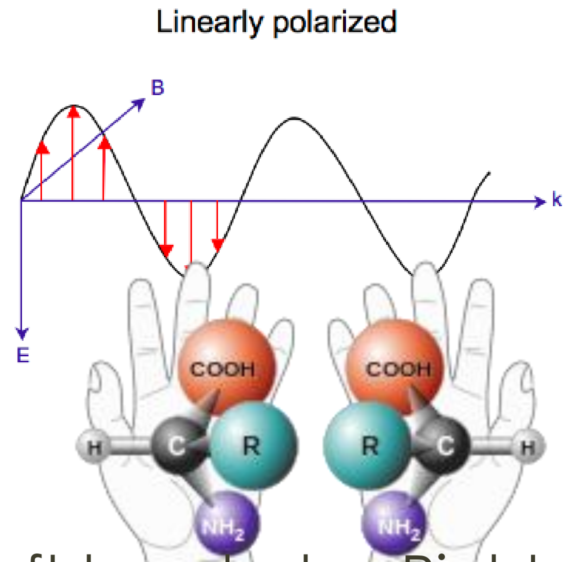


- Due to <u>Chirality</u>-
  Mirror Images not superimposable.
- **<u>Significance</u>**:
  - 3D information of molecules
  - Drugs can be poison if wrong `handedness'
  - Possible engineering of efficient solar energy cells[1-5]

1. http://www.ecs.soton.ac.uk/news/679
2. http://hdl.handle.net/2142/42174
3. Sabah, Uckun, J. Optoelectronics and Adv. Mat., Vol. 8, No. 5, pp.1918-1924, 2006.
4. Srivastava, et al., *Science*, 2010; 327 (5971): 1355.
5. Iowa Energy Center

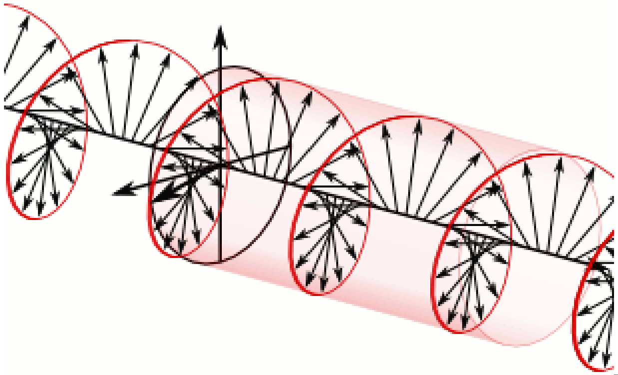
Light
= Electric Magnetic (EM) Field

1. Linear Polarization (**LP**)

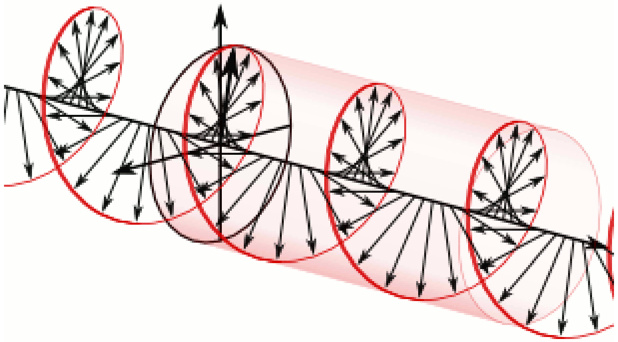


Left-handed or Right-handed molecules interact differently with LCP and RCP light

2. Left-Circular Polarization (**LCP**)

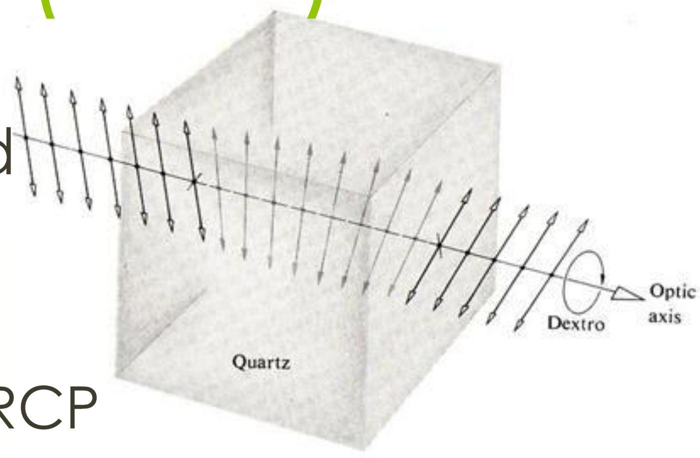


3. Right-Circular Polarization (**RCP**)



Optical Rotation (ORD)

- Rotation of Linearly Polarized light

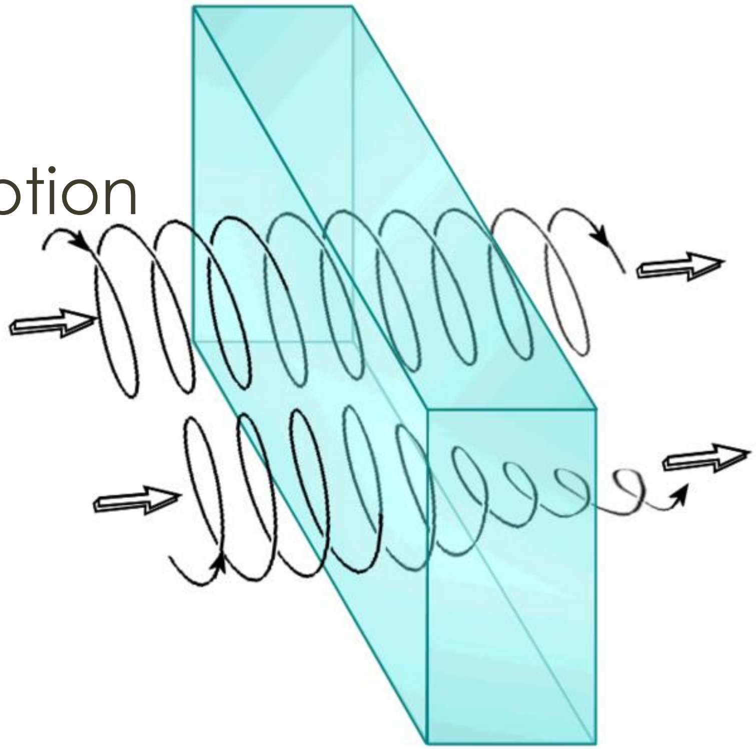


Because:

1. Linear Polarization = LCP + RCP
2. Left- and Right-Circular Polarized light rotate differently in chiral molecules

Circular Dichroism (**CD**)

- Absorption different for LCP and RCP in chiral medium
- Circular Dichroism = This Differential Absorption



Measuring Optical Activity

- Differential signals for left- vs. right-handed fields and molecules:
  - Very small ($10^{-6} - 10^{-3}$)
  - Difficult
- One measure is Dissymmetry Factor:

$$\mathbf{g} = \frac{A^L - A^R}{(A^L + A^R)/2} \sim \frac{\textbf{Circular Dichroism}}{\textbf{Average Absorption}}$$

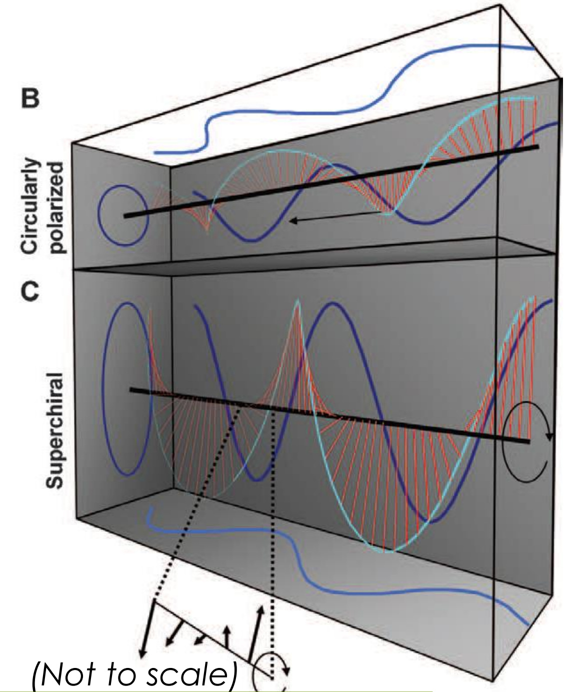
where A^L = LCP Absorption Rate, etc.

Part II: Limitations of a Superchiral Field

Choi, J. S. and Cho, M. *Physical Review A* **86**,063834 (2012)

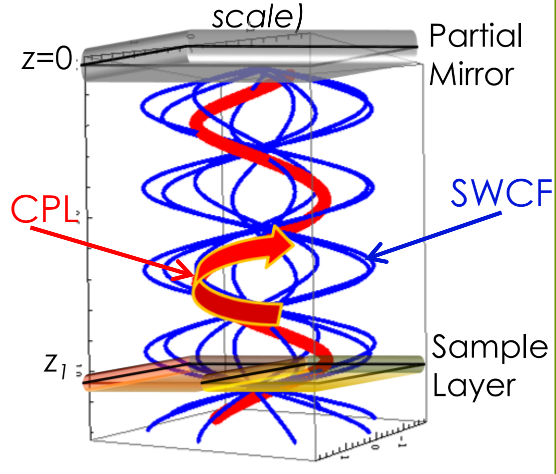
“Superchiral” Light

- Can we enhance Optical Activity signals dramatically?
- Y. Tang and A. E. Cohen, *Science* **332**, 333 (2011): Engineer light to increase Chirality
  - Create Standing Wave of RCPL + LCPL with mirror (**SWCF**)
  - Place Chiral sample at Electric Field Energy (U_e) Minimum (node)



(Not to scale)

(Sample size relative to field ~ to scale)



Cohen's "Superchirality"-Results

- Enhancement:

$$\frac{g}{g_{CPL}} = \frac{c\,C}{2\,\omega\,U_e} \rightarrow \frac{1+\sqrt{R}}{1-\sqrt{R}}$$

- R = Reflectivity of mirror
- "*Optical Chirality*":

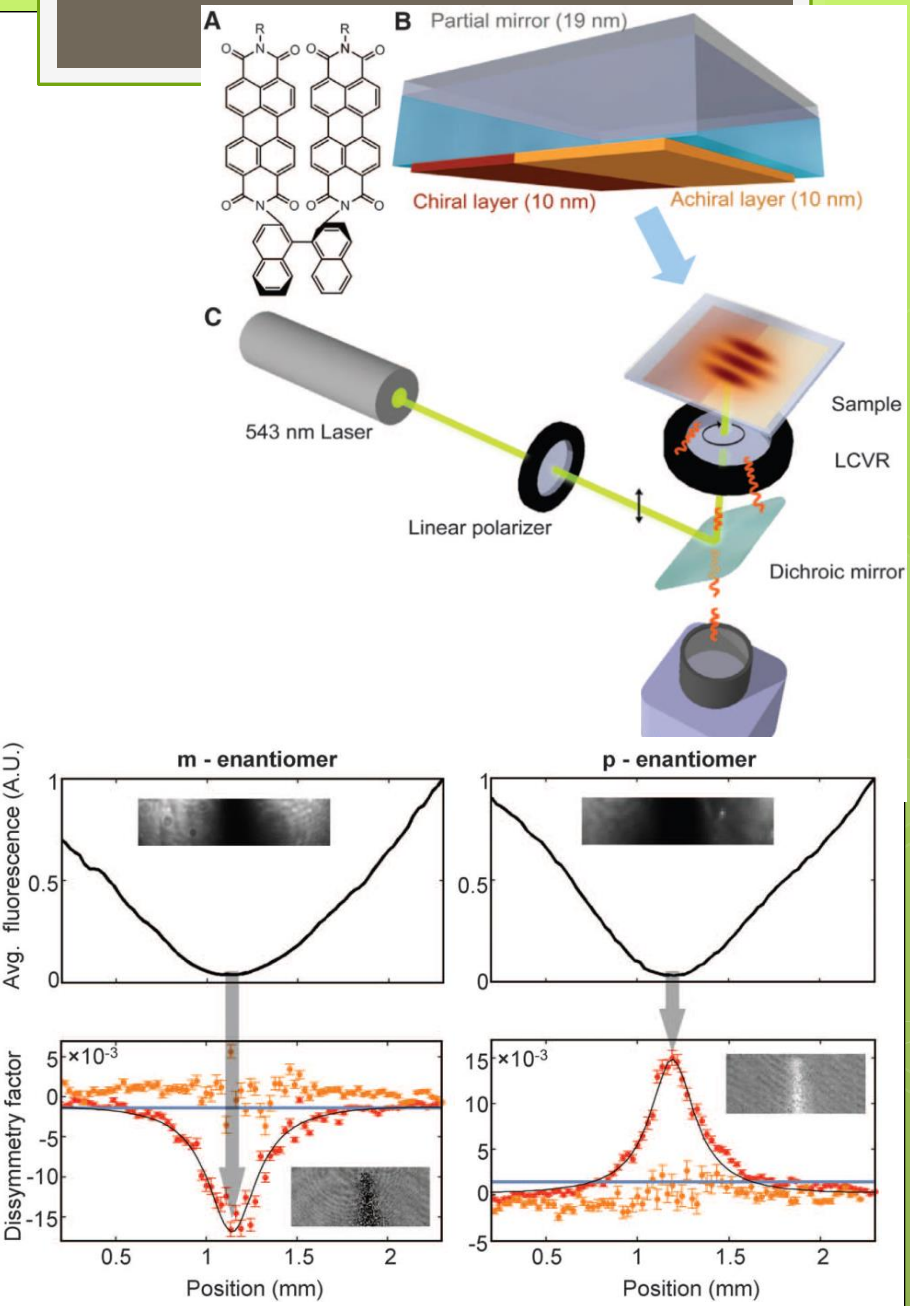
$$C \equiv \frac{\epsilon_0}{2}\mathbf{E}\cdot\nabla\times\mathbf{E} + \frac{1}{2\mu_0}\mathbf{B}\cdot\nabla\times\mathbf{B}$$

- For R=0.72:

11x enhancement

- For R=1:

Infinite enhancement?



WARNING- MATH FUN!

- Induced electric (p) and magnetic (m) dipole moments:

$$\tilde{\mathbf{p}} \simeq \tilde{\alpha}\tilde{\mathbf{E}} + \tilde{G}\tilde{\mathbf{B}}, \quad \tilde{\mathbf{m}} \simeq \tilde{\chi}\tilde{\mathbf{B}} - \tilde{G}\tilde{\mathbf{E}}$$

- Work done by EM fields:

$$W_{\mathrm{EM}} = \mathbf{p} \cdot \mathbf{E} + \mathbf{m} \cdot \mathbf{B}$$

- Total absorption rate of molecules:

$$A^{\pm} = \langle \dot{\mathbf{p}} \cdot \mathbf{E} + \dot{\mathbf{m}} \cdot \mathbf{B} \rangle_t$$

Generalized g for SWCF- Final

$$g = \left\{ \frac{(1-R)\left[4\gamma_{\text{ave}}^{\text{CPL}}\frac{n_{\text{ave}}^{0}\Delta n}{(n^2)_{\text{ave}}} + g_{\text{CPL}}\right]}{(1+R)\left[1+\gamma_{\text{ave}}^{\text{CPL}} + \frac{1}{2}g_{\text{CPL}}\frac{\Delta n}{n_{\text{ave}}^{0}}\right] + 2\sqrt{R}\left[\gamma_{\text{ave}}^{\text{CPL}}\frac{n^L n^R}{(n^2)_{\text{ave}}} - 1 - \frac{1}{2}g_{\text{CPL}}\frac{\Delta n}{n_{\text{ave}}^{0}}\right]\cos(2k_{\text{ave}}z)} \right\}$$

- Combined C_g, U_γ
- Calibrated amplitudes (R)
- Substituted with averaged parameters

$$g_{\text{CPL}} = -4\frac{G'(\text{g})n_{\text{ave}}^{0}}{\alpha'' c}$$

$$\gamma_{\text{ave}}^{\text{CPL}} \equiv \frac{\gamma^L + \gamma^R}{2}$$

$$\gamma^{(L/R)} \equiv \frac{(n^{(L/R)})^2\chi''}{c^2\alpha''} \geq 0$$

$$R \equiv (E_2/E_1)^2 = (E_2'/E_1')^2$$

$$n_{\text{ave}}^{0} \equiv \tfrac{1}{2}(n^L + n^R)$$

$$\Delta n \equiv \frac{n^L - n^R}{2} \quad (\Delta n : \text{positive or negative})$$

$$n^L = n_{\text{ave}}^{0} + \Delta n$$

$$n^R = n_{\text{ave}}^{0} - \Delta n$$

$$(n^2)_{\text{ave}} \equiv \frac{(n^L)^2 + (n^R)^2}{2}$$

$$k_{\text{ave}} \equiv \frac{k^L + k^R}{2} = \frac{\omega}{c}n_{\text{ave}}^{0}$$

g_0 for SWCF when Δn=0 (Simpler formula, good approximation)

$$g_0 \equiv g(\Delta n/n_0 = 0)$$
$$= g_{\mathrm{CPL}} \times \left\{ \frac{(1-R)}{(1+R)(1+\gamma_0) + 2\sqrt{R}(\gamma_0 - 1)\cos(2k_{\mathrm{ave}}z)} \right\}$$

- Drop γ_0 (10^{-6}-10^{-4})?
- No, or else same as Tang and Cohen.
- Write denominator differently -> U_e min => U_b max.

$$\{[\langle U_e \rangle_t] + \gamma_0[\langle U_b \rangle_t]\} \propto \left[(1+R) - 2\sqrt{R}\cos(2k_{\mathrm{ave}}z)\right] + \gamma_0 \left[(1+R) + 2\sqrt{R}\cos(2k_{\mathrm{ave}}z)\right]$$

Correcting Dissymmetry Factor (g)

- Conservation of Energy:

  Electric Energy(U_e) + Magnetic Energy(U_b) = Constant
- Before (for minimum U_e):

$$\frac{\mathrm{g}}{\mathrm{g}_{\mathrm{CPL}}} = \frac{c\,C}{2\,\omega\,U_e} \rightarrow \frac{1+\sqrt{R}}{1-\sqrt{R}}$$

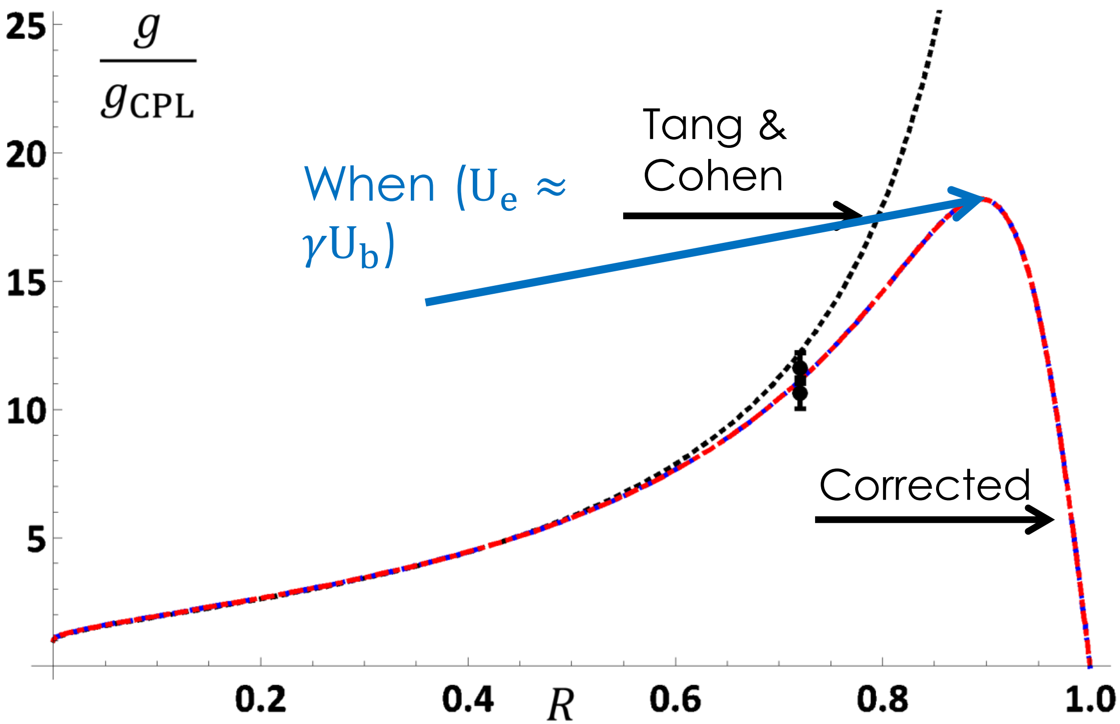
- Corrected (small $U_e \rightarrow$ large U_b)

$$g/g_{\mathrm{CPL}} = \frac{c\,C}{2\,\omega(\mathrm{U_e} + \gamma \mathrm{U_b})} = \frac{1-R}{(1-\sqrt{R})^2 + \gamma(1+\sqrt{R})^2}$$

  - $\mathrm{U_b}$ = magnetic field energy density
  - $\gamma \propto$ (magnetic susceptibility) / (electric polarizability)
  - γ = property of material; small; limits enhancement

Plot

1. Material (γ) fixes maximum enhancement (10x - 500x)
2. Find better material?
   But signal decreases faster than increase in enhancement



Conclusions 1

- Tang and Cohen:
  - Suggested simple and ingenious method
  - Renewed interest in C as physically useful quantity (discovered originally in 1964)
- We generalized Optical Chirality:

  $$C \equiv \frac{\epsilon}{2}\mathbf{E}\cdot\nabla\times\mathbf{E}+\frac{1}{2\mu}\mathbf{B}\cdot\nabla\times\mathbf{B},$$

  and analyzed optical rotation effects
- Our correction useful for ongoing discussion and future enhancement search

Acknowledgements 1

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