

Supplementary Information: Circular dichroism of relativistically–moving chiral molecules

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RESPONSE OF A MOLECULAR SYSTEM MOVING AT HIGH VELOCITY

A variant of the relativistic X2C transformation, taking into account the velocity of the system, has been considered to evaluate the molecular response of the system at high velocity. Following Ref. 1, we replace Eq. (14) therein by^{1,2}

$$\mathbb{K} = \begin{pmatrix} \mathbf{K} & \mathbf{0} \\ \mathbf{0} & 2c\sqrt{m} \sqrt{\frac{1}{\sqrt{1+\frac{v^2}{c^2}}}} \mathbf{K} p^{-1} \end{pmatrix}. \quad (1)$$

This transformation takes the velocity of the molecule itself into account, yielding the influence thereof on the molecular electron density. Subsequently, the response function is also altered. As shown by Fig S1 for chlorophyll *a*, however, the influence of approaching velocities at a fraction of the speed of light is negligible. There is barely any difference in the molecular response function at different velocities, making the this effect negligible. Assuming the molecular response function to be constant with increasing velocity therefore is an excellent approximation. This assumption can then conveniently be accessed simply from the non-relativistic calculation outlined by $c = \infty$ in Fig S1.

The simulations outlined in Fig. S1 have been carried out using the PBE0 functional^{3,4} in combination with the x2c-TZVPPall-2c basis set.⁵ A more extended basis set was chosen to ensure a higher flexibility upon the representation of the relativistic molecular transformation.

FAR-FIELD EXPANSION OF SCATTERED VECTOR SPHERICAL WAVES

In this section, we derive the far-field expansion of scattered vector spherical waves $|k'_s \ell' m' \lambda'_s\rangle$ used in the main article. Instead of the ket $|k'_s \ell' m' \lambda'_s\rangle$, we use the notation $\mathbf{W}_{\ell' m' \lambda'_s}^{(3)}(\mathbf{r}', k'_s)$ for the scattered vector spherical wave with wave number k'_s and helicity λ'_s . The vector spherical waves of well-defined helicity can be expressed as a sum of vector spherical waves of well-defined parity,

$$\mathbf{W}_{\ell' m' \lambda'_s}^{(3)}(\mathbf{r}', k'_s) = \frac{\mathbf{N}_{\ell' m'}^{(3)}(\mathbf{r}', k'_s) + \lambda'_s \mathbf{M}_{\ell' m'}^{(3)}(\mathbf{r}', k'_s)}{\sqrt{2}}, \quad (2)$$

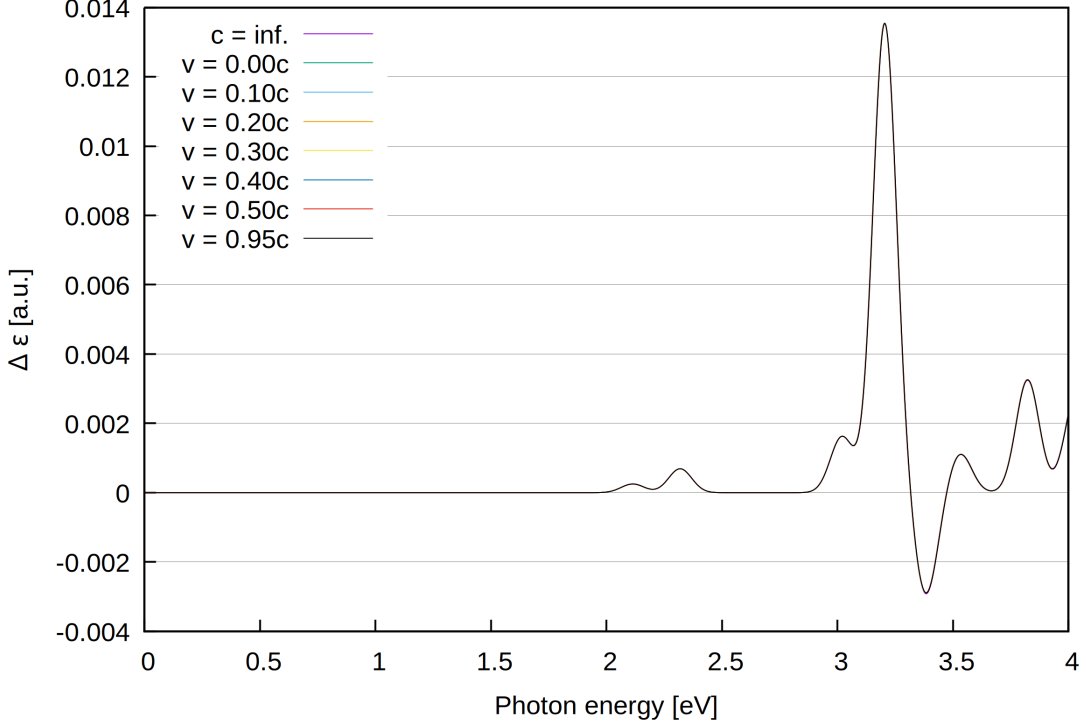


FIG. S1: Calculated circular dichroism spectra of chlorophyll *a* at velocities from $v = 0 - 0.95$ times the speed of light. The relativistic transformation outlined in Eq. 1 was used.

see equation (7) from⁶. $\mathbf{N}'_{\ell' m'}(\mathbf{r}', k'_s)$ corresponds to transverse magnetic (TM) modes and $\mathbf{M}'_{\ell' m'}(\mathbf{r}', k'_s)$ corresponds to transverse electric (TE) modes. With equations (11a) and (11b) from⁶, we have

$$\begin{aligned} \mathbf{M}'_{\ell' m'}(\mathbf{r}', k'_s) &= N_{\ell' m'} (\mathbf{i}\pi'_{\ell' m'}(\theta'_s) \hat{\theta}'_s - \tau'_{\ell' m'}(\theta'_s) \hat{\phi}'_s) e^{im'\phi'_s} h_{\ell'}^{(3)}(k'_s \mathbf{r}') = \mathbf{X}'_{\ell' m'}(\theta'_s, \phi'_s) h_{\ell'}^{(3)}(k'_s \mathbf{r}') \\ \mathbf{N}'_{\ell' m'}(\mathbf{r}', k'_s) &= \left[\mathbf{i}\sqrt{\ell'(\ell'+1)} Y_{\ell', m'}(\theta'_s, \phi'_s) \frac{h_{\ell'}^{(3)}(k'_s \mathbf{r}')}{k'_s r'} \hat{\mathbf{r}}' + \left(\frac{dh_{\ell'}^{(3)}(k'_s \mathbf{r}')}{d(k'_s r')} + \frac{h_{\ell'}^{(3)}(k'_s \mathbf{r}')}{k'_s r'} \right) \hat{\mathbf{r}}' \times \mathbf{X}'_{\ell' m'}(\theta'_s, \phi'_s) \right], \end{aligned} \quad (3)$$

where $\pi'_{\ell' m'}(\theta'_s) = \frac{m' P_{\ell'}^{m'}(\cos \theta'_s)}{\sin \theta'_s}$ and $\tau'_{\ell' m'}(\theta'_s) = \frac{\partial P_{\ell'}^{m'}(\cos \theta'_s)}{\partial \theta'_s}$, see equations (13a) and (13b) from⁶. $P_{\ell'}^{m'}(\cos \theta'_s)$ are the associated Legendre polynomials, see equation (B.2) from⁶, $Y_{\ell', m'}(\theta'_s, \phi'_s)$ are spherical harmonics, see equation (B.1) from⁶, and $N_{\ell' m'} = \mathbf{i}\sqrt{\frac{2\ell'+1}{4\pi\ell'(\ell'+1)} \frac{(\ell'-m')!}{(\ell'+m')!}}$ is a normalisation factor, see equation (12) from⁶. $h_{\ell'}^{(3)}(k'_s \mathbf{r}')$ are spherical Hankel functions of the first kind. In the limit of large distances, we derive

$$\mathbf{W}'_{\ell' m' \lambda'_s}(r' \rightarrow \infty, k'_s) = \left(\mathbf{Y}'_{\ell' m'}(\theta'_s, \phi'_s) (-\mathbf{i})^{\ell'} + \lambda'_s \mathbf{X}'_{\ell' m'}(\theta'_s, \phi'_s) (-\mathbf{i})^{\ell'+1} \right) \cdot \frac{\mathbf{e}^{\mathbf{i}k'_s r'}}{k'_s r'} \quad (4)$$

$$= \mathbf{Q}'_{\ell' m' \lambda'_s}(\theta'_s, \phi'_s) \cdot \frac{\mathbf{e}^{\mathbf{i}k'_s r'}}{k'_s r'}, \quad (5)$$

which is a vector in spherical coordinates. Here, $\mathbf{Y}'_{\ell' m'}(\theta'_s, \phi'_s) = \hat{\mathbf{r}}' \times \mathbf{X}'_{\ell' m'}(\theta'_s, \phi'_s)$. Multiplying the coefficient vector $\mathbf{Q}'_{\ell' m' \lambda'_s}(\theta'_s, \phi'_s)$ with the scattered vector spherical wave expansion coefficients $B'_{\ell' m' \lambda'_s}(k'_s)$, we have

$$\begin{pmatrix} E'_{s, \lambda'_s, r'_s} \\ E'_{s, \lambda'_s, \theta'_s} \\ E'_{s, \lambda'_s, \phi'_s} \end{pmatrix} = \frac{1}{k'_s r'} \sum_{\ell', m'} \mathbf{Q}'_{\ell' m' \lambda'_s}(\theta'_s, \phi'_s) B'_{\ell' m' \lambda'_s}(k'_s). \quad (6)$$

Note that the $1/k'_s r'$ component in equation (4) shows little variation for large r' , which allows us to consider the expansion coefficients on the left hand side of equation (6) in the plane wave basis.

DIRECTION AVERAGED TCD SIGNAL FROM MOLECULES

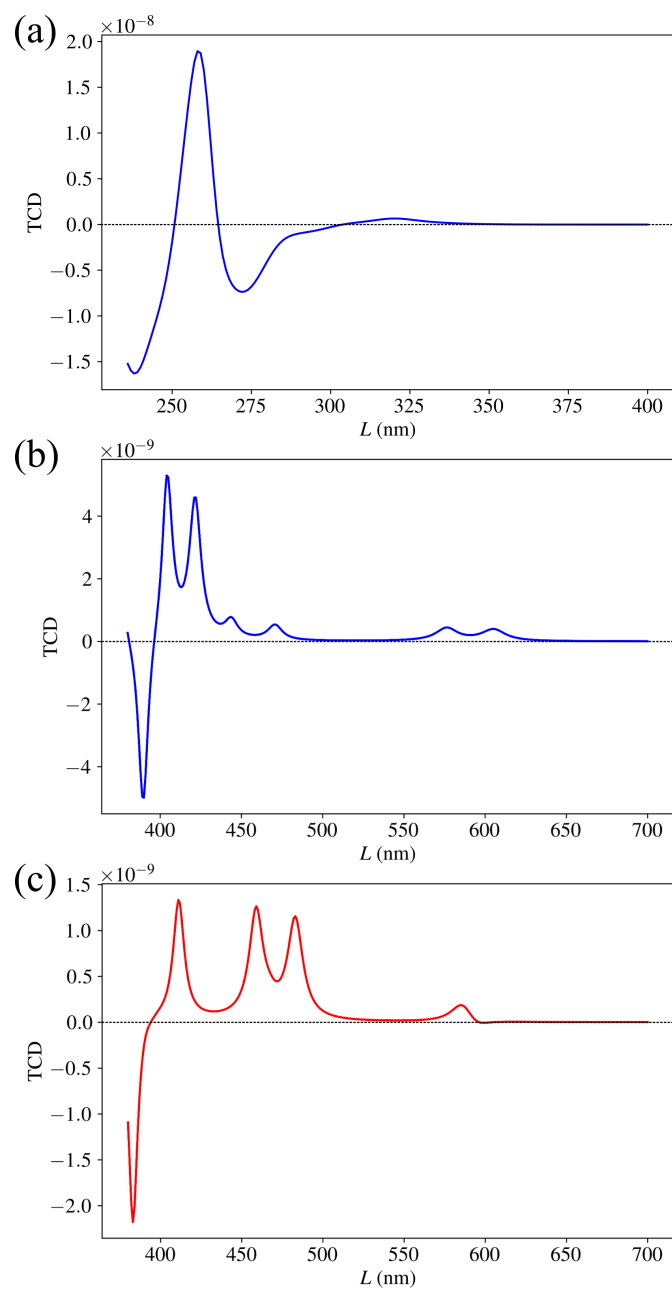


FIG. S2: Total TCD signal (with arbitrary scaling) scattered in all directions from the rotationally averaged (a) DNA molecular model; (b) Chlorophyll *a* and (c) Chlorophyll *b* molecules for speed ratio $\beta = 0$.

COMPUTATIONAL DATA FROM QUANTUM CHEMISTRY SIMULATIONS

All results of molecular quantum chemistry calculations can be found deposited to the NOMAD database for materials science under the following DOI: [https://doi.org/10.17172/NOMAD/2024.02.07-](https://doi.org/10.17172/NOMAD/2024.02.07-1)

1

AN EXAMPLE OF THE TURBOMOLE CONTROL FILE FOR ONE OF THE CALCULATIONS OF THE DYNAMIC POLARISABILITY TENSORS OF DNA MODEL

\$cosmo

epsilon= 78.355

rsolv= 1.30

refind= 1.3333

\$cosmo_atoms

radii in Angstrom units

c 1,3,5-7,9-11,15,22-23,25-27,29-30,32,34,36,44-45,47-49,51,53-54,56,58,65-66
68-70,72,74-75,77,79,86-87,89-91,93,95-97,103,106-107,109-111,113,115-117,
123,126-127,129-131,133,135-137,145-146,148-150,152,154-155,157,159,167,169
171-173,175-177,181,187-191,195,197-198,200,202,208-209,211-213,218,220-222
225,228-229,231-233,238,240-242,245,248-249,251-253,258,260-261,263,265,
269-270,272-274,279,281-282,284,286,290-291,293-295,300,302-303,305,307,
312-313,315-317,322,324-326

radius= 2.0000

n 2,4,20,28,31,33,35,38,50,52,55,57,62,71,73,76,78,83,92,94,112,114,132,134,
142,151,153,156,158,161,166,168,170,194,196,199,201,203,217,219,237,239,257
259,262,264,266,278,280,283,285,287,299,301,304,306,308,321,323,328

radius= 1.8300

o 8,12,14,16,18-19,21,24,37,39,41-43,46,59,61,63-64,67,80,82,84-85,88,98,
100-102,104-105,108,118,120-122,124-125,128,138,140-141,143-144,147,160,
162-165,174,178,180,182,184-186,192-193,204-207,210,214,216,223-224,226-227
230,234,236,243-244,246-247,250,254,256,267-268,271,275,277,288-289,292,296
298,309-311,314,318,320,327,329-330

radius= 1.7200
h 331-530
radius= 1.3000
p 13,17,40,60,81,99,119,139,179,183,215,235,255,276,297,319
radius= 2.1060
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\$cosmo_data file=cosmo_transfer.tmp
\$title
\$symmetry c1
\$coord file=coord
\$optimize
internal off
redundant off
cartesian on
\$atoms
basis =def2-TZVP
jbas =def2-TZVP
\$basis file=basis
\$scfmo file=mos
\$closed shells
a 1-1290 (2)
\$scfiterlimit 1000
\$scfdamp start=0.300 step=0.050 min=0.100
\$scfdump
\$scfdiis
\$maxcor 500 MiB per_core
\$scforbitalshift automatic=.1
\$energy file=energy
\$grad file=gradient
\$dft
functional pbe0
gridsize 3

```
$scfconv 7
$denconv 1.0d-7
$scftol 1.0d-15
$ricore 16000
$rij
$jbas file=auxbasis
$marij
$mgiao
$senex
gridsize 1
$esenex
$scfinstab dynpol nm
260
$damped_response 0.15 eV
$rpacor 140000 in_total
$scfiterlimit 300
$magnetic_response
$rundimensions
natoms=530
$last step mpshift
$end
```

CARTESIAN COORDINATES OF FINITE-SIZE DNA MODEL

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C 6.24597 3.2973 10.01367
N 5.90497 2.1383 10.63567
C 4.61797 1.8333 10.93067
N 3.64397 2.6963 10.61667
C 3.92597 3.8523 10.01167
C 5.23497 4.1943 9.68567
C 6.98697 1.2153 11.02367
```


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C 9.23197 1.4823 11.35967
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O 9.82997 -0.4417 10.04267
P 9.95797 -1.3387 8.73167
O 11.12897 -2.2157 8.87967
C 10.29297 2.5343 11.44967
O 9.96897 3.4953 10.44167
P 10.77297 4.8703 10.36667
O 12.21497 4.5653 10.33467
O 4.39397 0.7613 11.49667
N 2.92997 4.7483 9.74367
O 8.63997 -2.2137 8.78467
C 8.42297 -3.1257 9.86767
C 7.10197 -3.7907 9.61967
O 6.06197 -2.7987 9.61067
C 5.42497 -2.8497 8.33267
C 6.50197 -3.3827 7.40267
C 6.97297 -4.5217 8.29067
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C 5.46096 3.1943 -6.09433
C 6.92496 2.0823 -8.68533
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CARTESIAN COORDINATES OF CHLOROPHYLL A

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CARTESIAN COORDINATES OF CHLOROPHYLL *B*

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