Asymmetry of electron chirality between enantiomeric pair molecules and the origin of homochirality in nature

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(with K. Ito and T. Shimizu)

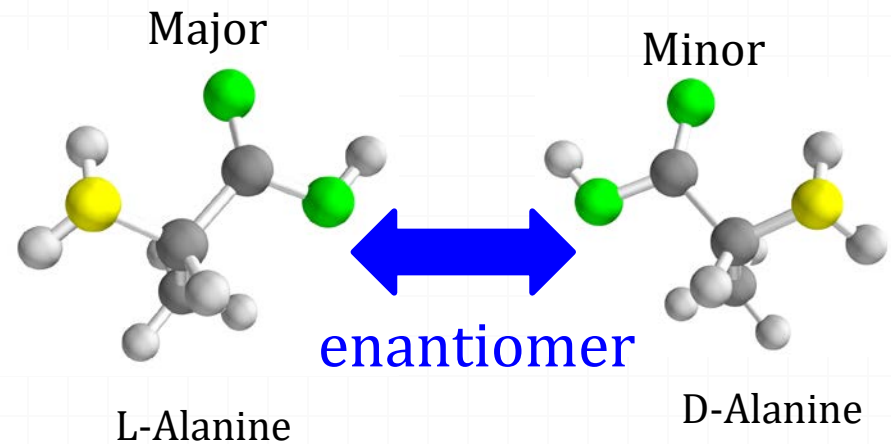Phys. Rev. A 99, 012509 (2019)
+ Preliminary results

Molecular parity violation

- Almost all biological molecules on the earth have strong chiral imbalance.
  - Amino acid : only L-chiral
  - Sugar : only D-chiral

  Homochirality

- The mechanism how this bias is generated is long-standing mystery.

Major

Minor

enantiomer

L-Alanine

D-Alanine

CORN rule
Carboxyl (CO), other (R), amino (N)
clockwise (D-chiral) or
counter clockwise (L-chiral)

Homochirality

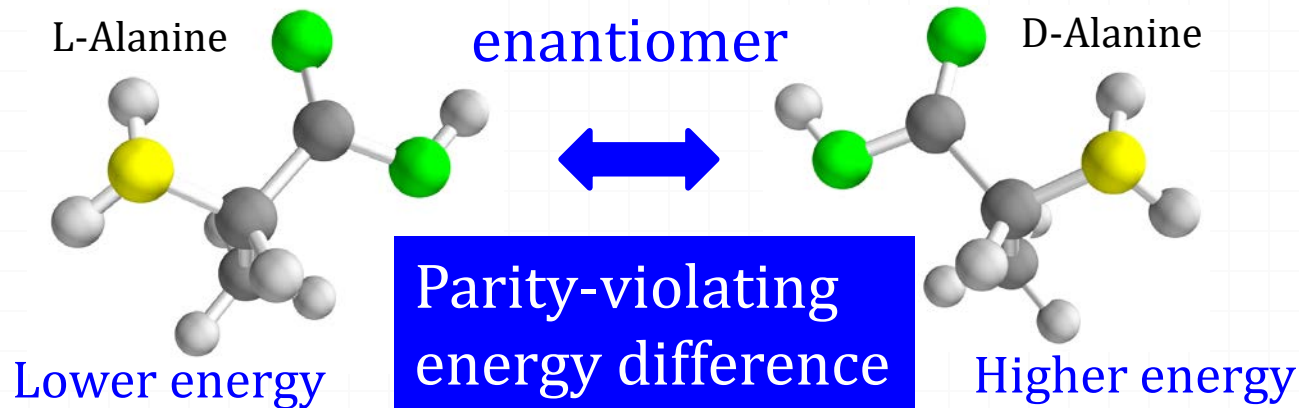○ The same amounts of L- and D-molecules are produced, without catalysis.

○ Homochirality is generated as:

Space or earth earth

1. **Parity symmetry breaking creates a small imbalance between enantiomers.**
2. **Chiral amplification** enhances imbalance to large bias and **Chiral transmission** may transfers this chirality to other enantiomers.

○ Salam proposed that parity-violating energy difference between chiral molecules generates the initial imbalance through phase transition such as crystallization.

Parity-violating energy difference

O The weak interaction between electrons and nuclei makes the energy difference between chiral molecules.

L-Alanine

enantiomer

D-Alanine

Parity-violating energy difference

Lower energy

Higher energy

$$E_{\mathrm{PV}} = \int d^3\vec{r}\,\langle\Psi|H_{\mathrm{PV}}|\Psi\rangle$$

$$= \frac{G_F}{2\sqrt{2}}\sum_n Q_W^n \sum_i \left(\int d^3\vec{r}\,\langle\Psi|\hat{\psi}_{e_i}^\dagger\gamma_5\hat{\psi}_{e_i}\hat{\psi}_{N_n}^\dagger\hat{\psi}_{N_n}|\Psi\rangle\right)$$

$$H_{\mathrm{PV}} = \sum_{i,n}\frac{G_F}{2\sqrt{2}}Q_W^n\hat{\psi}_{e_i}^\dagger\gamma_5\hat{\psi}_{e_i}\hat{\psi}_{N_n}^\dagger\hat{\psi}_{N_n}$$

Other possibility

0 Parity-violating energy difference between enantiomers is supposed to be too small. (typically 10^{-19}eV)

0 Some other mechanism are proposed and discussed.

   0 Circularly polarized light may trigger the formation of an enantiomeric excess in space.

   0 Electrons (and others) from beta decay generates circularly polarized bremsstrahlung photons (Vester-Ulbricht hypothesis).

   0 and so on.

0 However, not settled yet.
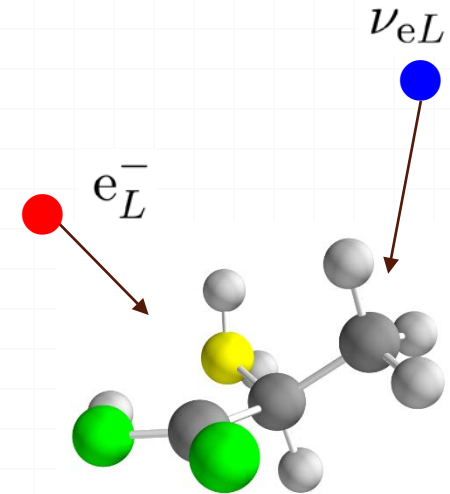
Total electron chirality of molecule?

0 Nonzero E_{PV} → nonzero electron chirality at nuclei

0 Question: Is total electron chirality is zero or not?

  0 Parity symmetry is violated in chiral molecules.

  0 Electron chirality can be flipped by electron mass.

0 Total electron chirality
  has not been paid attention

  0 Only one paper reported total chirality
    of H_2Te_2 in addition to studying E_{PV}.

Chiral molecule

Nuclei

Nonzero
electron
chirality
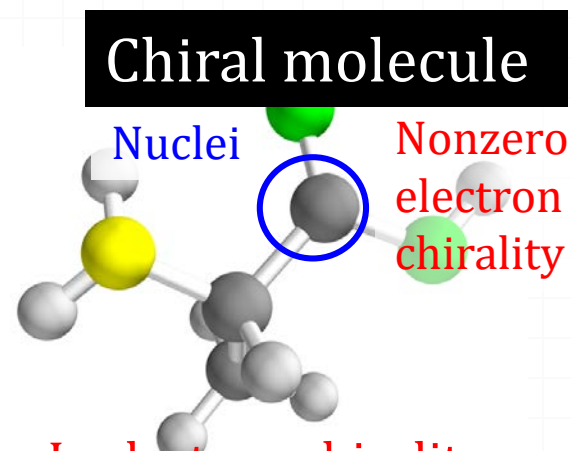
Is electron chirality
nonzero after integration
Over whole molecule?

Our proposal for homochirality

O If total electron chirality is nonzero in chiral molecules,

    O left-handed electron number is different between both enantiomers.

O Left and right-handed (chiral) electrons have different charge of the weak interaction.

O The weak interaction (e.g. beta decay)

    O Violate Parity symmetry

O We have proposed a new scenario.
If total electron chirality in enantiomers is nonzero, one enantiomer of a chiral molecule may be more lost by the weak interaction with other particles in space and/or on the earth slightly than the other enantiomer.

ν_{eL}

e_L^-

Our work:

We confirm that total electron chirality of chiral molecules is nonzero.
This nonzero electron chirality contributes to the homochirality in Nature.

Computational detail

H_2X_2

X=O, S, Se, Te

O Molecules:
  O H_2X_2 (X=O, S, Se, Te)
  O Amino acid (Alanine, Serine, Valine)
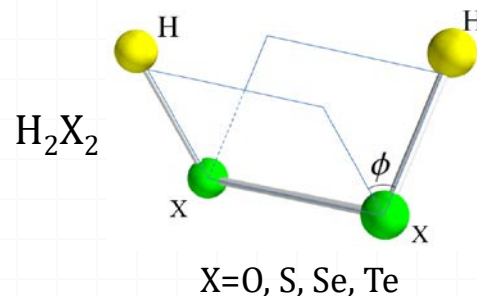O Electronic structure computation
  O DIRAC14 (public code)
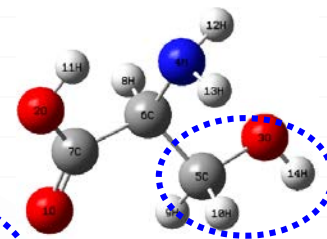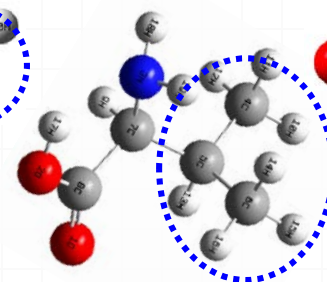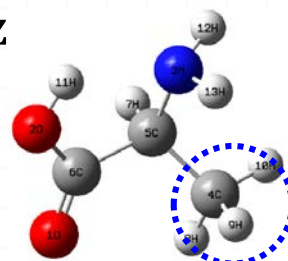 O Basis set: dyall.ae4z, aug-ccpv6z
  O Hartree-Fock with
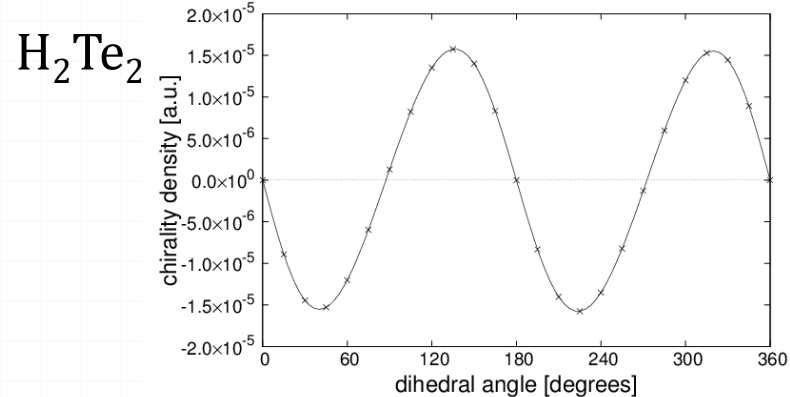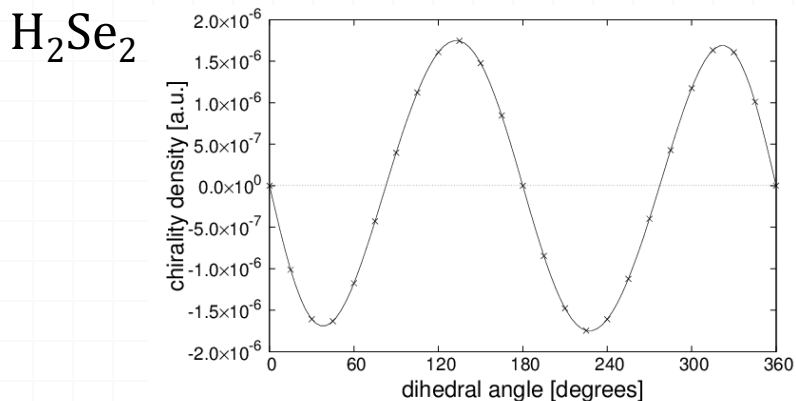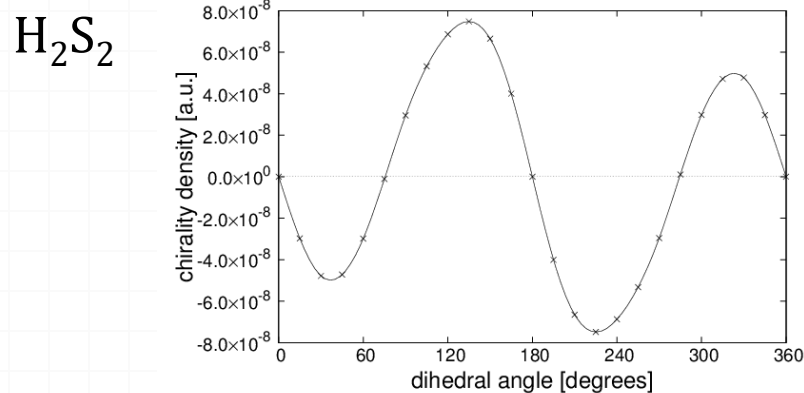   Dirac-Coulomb Hamiltonian
O Other computations
  O QEDynamics

L-Alanine

L-Valine

L-Serine

Total chirality

H_2O_2

preliminary

H_2S_2

H_2Se_2

H_2Te_2

H_2Te_2 is consistent with the result of other group,
while for other molecules any groups do not reported any results
Total chirality should have the same dependence on dihedral angle.
The structure of molecules governs the amount of total chirality by spin-orbit interaction.
The values are larger for heavier nucleus due to larger spin-orbit interaction

H_2Te_2

- Contributions from each orbital
  - Contribution from a high-energy orbital is larger than total chirality.
 - Small total chirality is derived as cancellation between contributions.

- Excitation gives larger total chirality?
- We confirmed that this cancellation is broken in ionized state.

No.	E_i [a.u.]	$\psi_i^\dagger \gamma_5 \psi_i (\vec{r}_{Te})$	$\int \psi_i^\dagger \gamma_5 \psi_i dx$
41	-1.936	4.150×10^{-6}	-1.440×10^{-5}
42	-1.934	-4.090×10^{-5}	2.410×10^{-5}
43	-1.927	8.520×10^{-5}	-2.230×10^{-5}
44	-1.926	-5.380×10^{-5}	1.180×10^{-5}
45	-1.923	7.100×10^{-5}	-3.590×10^{-6}
46	-1.922	-7.400×10^{-5}	4.600×10^{-6}
47	-0.866	-8.140×10^{-4}	5.950×10^{-7}
48	-0.764	-3.350×10^{-4}	6.300×10^{-7}
49	-0.513	-2.860×10^{-3}	-1.060×10^{-6}
50	-0.461	-1.490×10^{-2}	2.010×10^{-5}
51	-0.396	9.460×10^{-2}	-1.010×10^{-4}
52	-0.358	-8.950×10^{-2}	1.260×10^{-4}
53	-0.301	1.990×10^{-3}	-5.240×10^{-5}
total		-2.584×10^{-2}	-1.530×10^{-5}
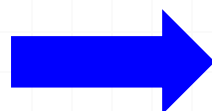
H_2Te_2 : -1.530×10^{-5} ⟶ $H_2Te_2^{2+}$: 1.891×10^{-4}

Doubly ionized molecule is probably unstable due to the reduction of electrons forming covalent bonds. This result is only for the purpose of demonstration

Amino acid

- Right-handed electron is more major in L-chiral alanine.

- D-chiral alanine may be more fragile for the weak interaction

- Our results indicate that this value is enhanced by ionization.

Molecule	Basis set	Total Chirality
L−Alanine	dyall.ae4z	6.85×10^{-10}
L−Alanine^{2+}	dyall.ae4z	-1.21×10^{-9}
L−Serine	dyall.ae4z	2.42×10^{-9}
L−Serine^{2+}	dyall.ae3z	-2.04×10^{-8}
L−Valine	dyall.ae4z	9.82×10^{-11}
L−Valine^{2+}	dyall.ae3z	2.50×10^{-8}

Summary

O Electron chirality in chiral molecules

   O Chiral molecules have nonzero total chirality of electrons.

      Molecular chirality generate electron chirality

   O This may be the origin of the homochirality, because nonzero total chirality of electrons induces different rate of weak interaction between two enantiomers.

   O The value of total chirality in a chiral molecule is drastically changed if the molecule may be ionized or excited.

O To do

   O What processes are important? Ionization? Other processes?

   O Which particles? Neutrino or electron?

   O Fluxes of those particles?   Cross section?