A Digital Twin in the Context of Photonic Material Design

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if not Tcyl.helicity:
    Tcyl.changebasis()
for ith in range(len(theta_x.flat)):
    kxwave = k0np.sin(theta_x.flat[ith])
    kywave = k0np.sin(theta_y.flat[ith])
    kparwave = np.array([kxwave, kywave])
    kpars = kparwave + ptsa.lattice.diffr_orders
    Qarray = ptsa.QMatrix.array(Tcyl, kpars, a)
Motivation

Chiral molecule
= no mirror symmetry

Left-handed enantiomer

Right-handed enantiomer

Examples:
Most amino acids & other biomolecules
Many drug / medicinal molecules
Motivation

Chiral molecule
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Optical measurement of chirality

Problem:
Chirality of molecules is weak
Solution:
Nanophotonic enhancement
Digital twin
Quantum chemistry calculations & nanophotonic enhancement

Density functional theory

Molecule

Electrons

Vibrations
Quantum chemistry calculations & nanophotonic enhancement

Density functional theory

Molecule

Electrons

Vibrations

Traditional measurement

Measurement using a photonic cavity
Quantum chemistry calculations & nanophotonic enhancement

Density functional theory

Molecule

Electrons

Vibrations

Traditional measurement

Measurement using a photonic cavity
Predicting measurement results & analyzing the data

Example of enhanced measurement
Predicting measurement results & analyzing the data

**Example of enhanced measurement**

- 50x enhancement of signal by photonic cavity
- Spectrum of molecules (not to scale)

**Determining the enantiomer**

- Calculated spectra (clean)
- Experimental spectra (noisy)

\[ \int s(\lambda)s_{\text{ref}}(\lambda) d\lambda \rightarrow \text{LH} \]
\[ \int s(\lambda)s_{\text{ref}}(\lambda) d\lambda \rightarrow \text{RH} \]
Conclusions

• Digital twin approach allows us to:
  • Accurately determine molecules’ quantum-mechanical properties
  • Design a device that makes measurements of molecular chirality faster
  • Predict and analyze the results of a real-world experiment

• Future work
  • Experimental realization

• Impact
  • 50 – 1000 faster measurement, or being able to measure smaller concentrations
  • Laboratory experiment, production