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# A Digital Twin in the Context of Photonic Material Design

## **Markus Nyman**

Co-authors: Xavier Garcia-Santiago, Marjan Krstić, Ivan Fernandez-Corbaton, Martin Wegener, Willem Klopper, Carsten Rockstuhl



HELMHOLTZ

### Introduction



#### HELMHOLTZ

### **Motivation**

Chiral molecule = no mirror symmetry



Left-handed enantiomer Right-handed enantiomer

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

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# Optical measurement of chirality





Problem: Chirality of molecules is weak Solution: Nanophotonic enhancement

### Digital twin



#### HELMHOLTZ

### Quantum chemistry calculations & nanophotonic enhancement



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### Quantum chemistry calculations & nanophotonic enhancement



### Predicting measurement results & analyzing the data

### Example of enhanced measurement



### Predicting measurement results & analyzing the data



### 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