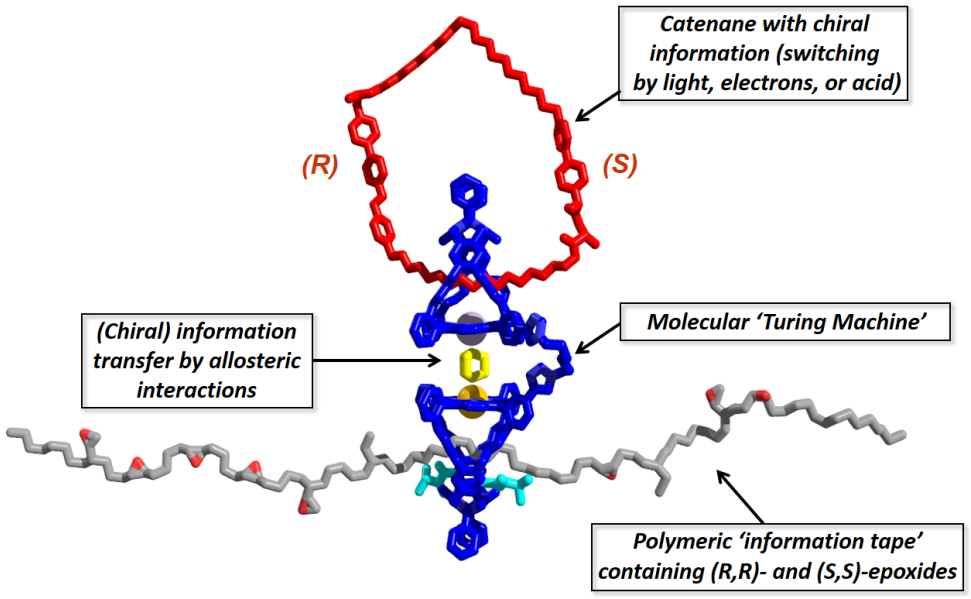
# The Molecular Nanotechnology Group

**Dr. Hans Elemans – group leader**

## The big picture

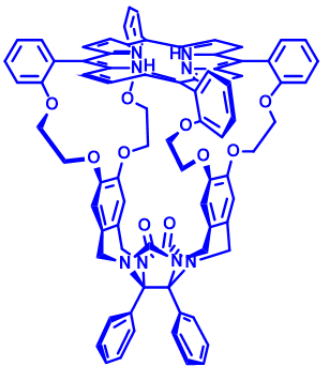
Our group aims at developing new and sustainable technologies to write, store, and read information onto molecules, more specifically polymer chains. For this we use synthetic molecular machines that are inspired by the **Turing machine**, a hypothetical device proposed by the British mathematician Alan Turing in 1936 as the general basis for the operation of a computer. Data storage on polymers (*Nature Rev. Chem*. 2018, doi.org/10.1038/s41570-018-0051-5) is highly relevant nowadays, as it is seen as a first step to solve the future problem of handling the exponential growth of information that is currently trafficking the internet. Moreover, molecular data storage is expected to demand orders of magnitude less energy than conventional data storage in large data centers.




## Processive catalysis

We are inspired by how nature controls the modification of biopolymers as molecular data storage materials, using so-called **processive enzymes**. These cavity-containing catalysts wrap themselves around a polynucleotide substrate, similar to a thread passing through a needle, and carry out many rounds of catalysis without dissociating from the substrate. In this manner, DNA is replicated extremely efficiently, reliably and rapidly by the enzyme DNA-polymerase, or degraded by the enzyme λ-exonuclease.

In 2003 our group was the first to develop a **synthetic processive catalyst**, consisting of a macrocyclic metal-porphyrin cage that threads a polybutadiene chain through its cavity and converts its alkenes to epoxides (*Nature* 2003, doi.org/10.1038/nature01925; *Science* 2008, doi.org/10.1126/science.1164647; *Chem. Eur. J.* 2024, doi.org/10.1002/chem.202304230). The **porphyrin cage**, a synthetic cavity molecule with a catalytic porphyrin 'roof', is the working horse in our group. It is obtained via an 8-step synthesis, contains a rigid cavity of about 1 nm diameter, can bind various transition metals in its porphyrin, and acts as a supramolecular host for the binding of guest molecules via non-covalent interactions (*Chem. Commun*. 2019, doi.org/10.1039/c9cc04372a).

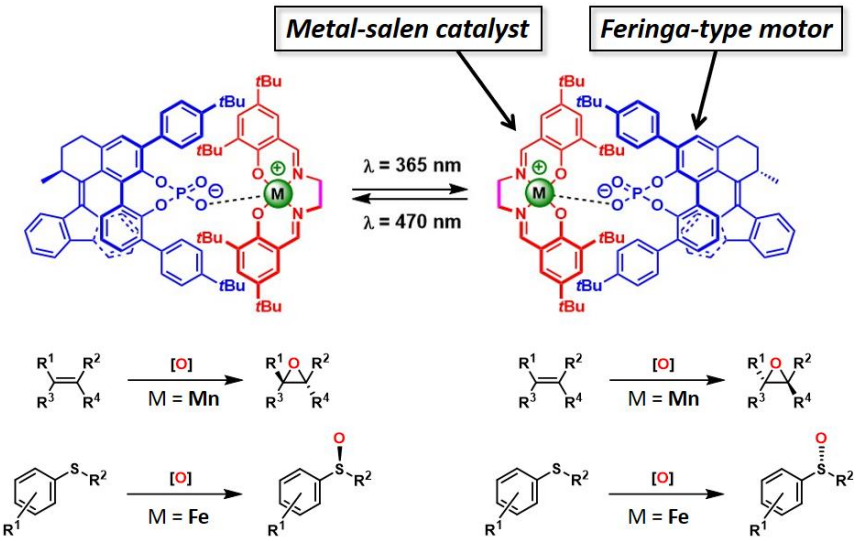


***Porphyrin cage***

## Current research in the group

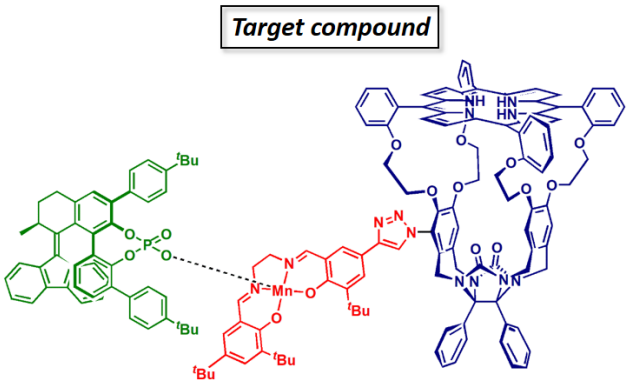
Our aim is to use our porphyrin cage as a **molecular Turing machine** (*Chem. Sci.* 2015, doi.org/10.1039/c5sc02317c). First, we aim to use the cage as a processive catalyst that can 'write' binary codes in the form of (*R,R*)- and (*S,S*)-epoxides or (*R*)- and (*S*)-sulfoxides on a polymer substrate that threads through the cavity. The two enantiomers of the chemical functionalities then represent the digits 0 and 1. For this to succeed, we need to meet two requirements:

- The polymer chain should move in one direction through the catalytic porphyrin cage in order to control the sequence of the code (**unidirectionality**).
- The catalytic function of the porphyrin cage should be switchable, so that it can 'write' both enantiomeric epoxides or sulfoxides on the chain (**enantiodivergence**) in a precisely controlled fashion.




Although achieving unidirectional motion remains a big challenge, we have recently succeeded in controlling the enantioselectivity of a single catalyst to catalyze the formation of both enantiomers of an epoxide from an alkene substrate, or both enantiomers of a sulfoxide from a sulfide substrate. For this, we employed a metal-salen complex to which a **Feringa-type molecular motor** is coordinated. With two different wavelengths of light, the motor can be reversibly switched between two pseudo-enantiomeric configurations. These opposite chiralities then allow the complex to catalyze the formation of opposite enantiomeric products in an epoxidation or a sulfoxidation reaction (*Nature Synth.* 2022, doi.org/10.1038/s44160-022-00157-7; *Chem. Eur. J.* 2023, doi.org/10.1002/chem.202203539).

**Current research in our group** focuses on combining the enantiodivergent metal-salen-motor conjugates with the porphyrin cage, by covalently connecting them via click chemistry. With the resulting target compounds, we aim to thread polymeric olefins or sulfides through the cage and convert them unidirectionally and enantiodivergently into chiral epoxides and sulfoxides.




## Internship opportunities

The research you can conduct in our group can be highly diverse:

- **Multistep synthesis** of complex (metal-)organic molecules, such as (metal-)porphyrin cages, light-switchable Feringa-type molecular motors, metal-catalysts, oligomers and polymers, and their characterization with various techniques (NMR, IR, circular dichroism, UV-vis and fluorescence spectroscopy, mass spectrometry).
- **Physical organic chemistry** measurements: host-guest binding thermodynamics, polymer threading kinetics, light-switching of molecular motors, unraveling reaction mechanisms.
- Supramolecular and processive **catalysis** experiments using the abovementioned molecules.

As an internship student (bachelor or master) you may choose to work on each of these topics, or on a combination of them. Depending on the current state of play, specific internship topics may vary on a month-to-month basis. **If you are interested in an internship in our group, please contact me (J.Elemans@science.ru.nl) for an appointment and I will be happy to give you more information about the possibilities.**