# Unravelling and optimizing the photoisomerization dynamics of light-driven molecular rotary motors

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## Abstract for the general public

One of the most challenging tasks for the progress of mankind is the construction of nanometer-sized devices, generally called molecular machines. These sophisticated devices are molecular structures capable of performing specific functions in a controlled manner. Inspired by nature's motor proteins (e.g. ATP synthase, kinesine and myosine), scientists have developed the first artificial prototypes of molecular machines, such as molecular shuttles, scissors, valves, and muscles. Key components of these artificial nanoscale machines are molecular motors, i.e. molecules or molecular assemblies converting the energy supply into mechanical motion. One of the most promising class of molecular motors are the so-called light-driven molecular rotary motors, which convert light energy into unidirectional rotational movement. The use of light to drive molecular motors is inherently advantageous due to its ability to impart high spatio-temporal control, without formation of waste products, and can be exploited for applications in different fields, such as material science, catalysis and biomedicine. The first synthetic light-driven molecular motor was introduced in 1999 by the Nobel laureate Feringa and coworkers, who then rapidly progressed in their research work and realized different families of molecular rotary motors. In these molecules, the 360° rotational motion of one moiety with respect to the rest of the molecule is achieved through four consecutive steps: two energetically uphill light-driven reactions, called photoisomerizations, and two energetically downhill thermal steps. While detailed understanding of the thermal steps has been achieved, the light-driven reactions of molecular motors are not yet fully understood. In this project, we intend to unravel the elusive light-driven reactions of Feringa's molecular motors by performing computational simulations. Our research study will allow to better understand and interpret the experimental observations for the investigated motors, as well as to develop a relationship between molecular structure and light-induced behaviour of molecular motors. Moreover, the knowledge acquired from our simulations will be exploited to propose new strategies to improve the efficiency of light-driven reactions in Feringa's molecular motors. Enhancing the efficiency of molecular motors is of paramount importance to reduce the undesired dissipation of light energy as heat in molecular machines.