New molecular spin qubits connected with photoswitchable diarylethenes for the construction of quantum computers

Quantum computers appear to be the next milestone that will take modern technology to the next level. Despite the advanced technologies implemented in supercomputers, they still cannot cope with complex computational problems involving many variables and interactions such as modelling the behaviour of atoms within larger molecules. Regardless of the computing power of supercomputers, they will not be able to solve such problems in a finite amount of time. Hence the enormous motivation and determination of scientists to create quantum computers, which thanks to quantum physics, will be able to cope with such complex problems.

The building blocks of quantum computers are qubits - the equivalent of bits in standard devices. Qubits, unlike bits, can exist in superposition in two states $|0\rangle$ and $|1\rangle$,, making them work on the principles of quantum physics and a better ‘tool’ for solving complex calculations.

In the project presented here, the main objective will be to obtain qubits based on lanthanide complexes that can be modified using light, by attaching photochromic compounds - diarylethenes - to the metal atom. Adding functionality such as photoswitchability to the qubits will enable faster recording of information using light, a highly desirable feature for quantum computers. Currently, light-responsive compounds have found widespread applications, such as in eyeglasses that dim when exposed to sunlight, which is reversible when entering a darker room.

The ongoing project consists of three main stages. Firstly, molecular qubits based on lanthanide complexes combined with photoconvertible diarylethenes will be designed to retain the desired properties. This part resembles the work of a designer who, using the appropriate building blocks, in this case chemical molecules, designs the target system - the qubits. Then, in the second stage, we move on to laboratory work, where the conditions must be chosen in such a way that the designed molecules can be obtained - this is the most demanding part because of the work with new, previously undescribed molecules, which sometimes makes it difficult to predict how they will behave. The third - and final - stage involves characterising and studying the properties of the resulting complexes. First, it is necessary to ‘grow’ a crystal of the compound obtained and X-ray it, thanks to which we are able to study its structure in detail. Then, the compound obtained is examined using available methods in order to gain a thorough understanding of its characteristics.

The fundamental research that takes place during this project allows us to gain a better understanding of the matter around us, at the level of single-particle behaviour, which has the potential to be used in quantum computers.