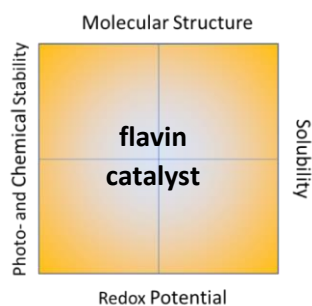


The main aim of the project is to formulate the general design principles and guidelines to build sustainable high-performance flavin derivatives suitable for future practical use in photocatalysis, taking into account their most fundamental properties, which include appropriate molecular structure and photophysical properties, redox properties, solubility and photo- and chemical stability.



Visible-light photocatalysis is in the forefront of interest as it allows new chemical transformations not accessible by conventional methodologies. One of the most promising classes of organic photocatalysts are flavins derived from prominent natural chromophores like FMN and FAD. Despite great attention, the research on applications of flavins in organic photocatalysis faces several challenges, such as chemoselectivity, absorption in visible spectral range, photochemical stability, appropriate redox properties, triplet excited state energy and production of singlet oxygen.

The objectives are to be achieved through international cooperation of a group skilled in flavin synthesis and photocatalysis with a group focused on photo-physics and quantum chemical calculations.

Within the project, three specific tasks to overcome above-mentioned challenges will be solved;

Task 1 - Tuning reactivity of flavins in oxidations (towards chemoselectivity).

Task 2 - Towards flavin photocatalysis with low-energy light (towards red).

Task 3 - Flavins regeneration/stability (towards stability).

Following deliverables are expected at the end of the project:

1. Library of 25 dyes fully characterized chemically and spectroscopically.
2. Library of 20 systems for catalytic purpose fully characterized chemically, morphologically and spectroscopically
3. Structure vs properties relationship in at least 4 series of flavins.
4. New efficient flavin-based catalytic systems (no less than 4) for use in organic synthesis.
5. Extension of the range of dyes to the Vis range spectrum (above 380 nm).
6. Elaboration of a list of critical elements required for efficient flavin type catalyst.
7. General instructions for flavin-catalyst design.