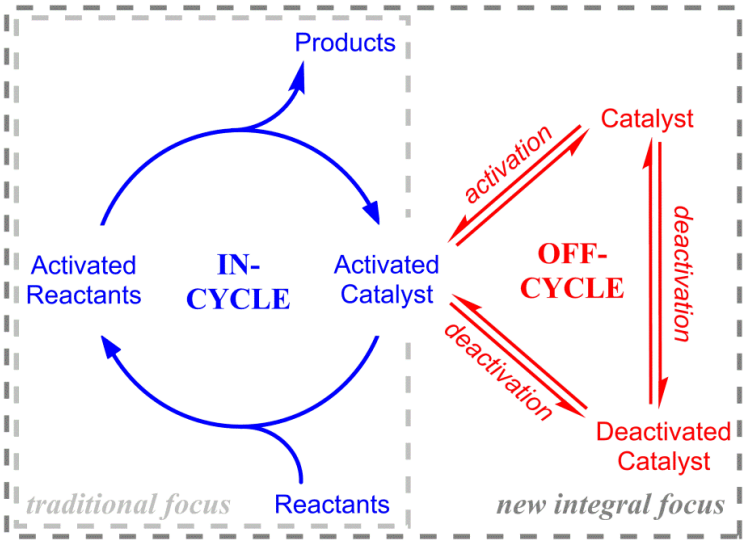
A computational approach to catalytic water oxidation and carbon dioxide reduction as new energy sources

Motivation and challenge. One of the main challenges faced by modern societies is the generation of energy from renewable sources in an environmentally-friendly manner. Two of the most promising approaches are carbon dioxide reduction (CDR) to methanol and water splitting (WS) to oxygen and hydrogen.

Objectives and scope. Both CDR and WS require catalysis due to their high activation energies. The catalysts available to date require further optimization in terms of activity, robustness and sustainability. This challenge will be tackled by using state-of-the-art computational methods. These will be applied to determine the properties, including structures and energies, of the intermediates and transition states involved in the catalytic cycle. A novel approach focusing on both in- and off-cycle steps (see Figure) will be used. The aim is to identify the critical steps and to use the insight provided by the calculations for a rational approach to enhanced catalytic systems. This project will involve close collaborations with research groups in the USA, including those led by Profs. Bernskoetter (Brown University) and Crabtree (Yale University).



Skills to be developed.

- Computational methods (geometry optimization, molecular modelling, Gaussian09, etc.)
- Data analysis (collecting and plotting data, electronic structure analysis, etc.)
- Communication (writing reports and drafts, oral presentations, Skype meetings, etc.)

Contact information. Co-supervised by Ainara Nova (ainara.nova@kjemi.uio.no, office V220, tel. 22858149), David Balcells (david.balcells@kjemi.uio.no, office V228, tel. 22857255) and Mats Tilset (mats.tilset@kjemi.uio.no, office at inGAP, tel. 22855502).