EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

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COST Action CM1205

Catalytic Routines for Small Molecule Activation (CARISMA)

2013 | 2017

Objectives

- To attain a fundamental understanding of the catalytic principles involved in the transition metal-catalyzed activation of small molecules through concerted research activities in silico and in vitro, and using an integral approach to catalysis.
- To development of an integral model of catalytic reactivity through computational models and mechanistic elucidations to deduce concepts to reliably anticipate the catalytic activity of transition metal complexes and verification of these concepts experimentally.
- To boost catalytic performance through application of these integral models.
- Anticipated Impact on different levels through delivering novel technologies with broad implications: (i) efficient reduction of greenhouse gases and selective incorporation into value-added products; (ii) increasing the hydrogen economy and the availability of solar fuels; (iii) new synthetic tools from using abundant feedstocks.

Main Achievements

- Kick-off meeting on May-22, 2013, formal launch of Action on June-2.
- Enthusiastic coordinators of WGs appointed.
- First Action meeting (MC and WGs) planned for autumn 2013.

Chemistry and Molecular Sciences and Technologies (CMST)

Participating countries

CH, DE, DK, ES, FR, HU, IS, IT, IE, NL, NO, PL, PT, SK, SI, SE, TR, UK

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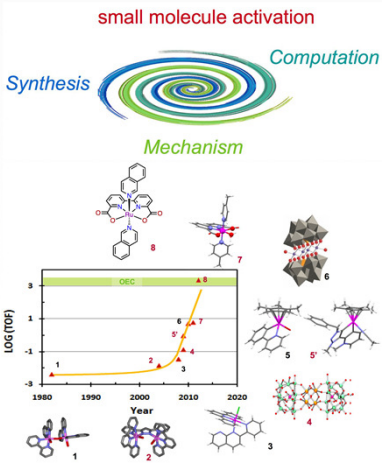

Interplay of synthetic, mechanistic, and computational expertise to boost catalytic activity.

COST is supported by the EU RTD Framework Programme

ESF provides the COST Office through a European Commission contract

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Working Group activities

Working Group 1

- Nitrogen-based redox chemistry:
  develop expertise in the synthesis, mechanistic understanding, and improved activity of transition metal catalysts for the fixation and activation of N_2 and NH_3.

Working Group 2

- CO_x activation and transformation:
  Generating, understanding, and improving transition metal catalysts for the fixation and reduction of CO_2 and CO for energy storage and for providing new synthetic C_1 synthons.

Working Group 3

- Oxygen-based redox chemistry:
  Improve the mechanistic principles of H_2O and O_2 binding and activation at transition metal catalysts and improving the catalytic activity for H_2O oxidation and O_2 cleavage.

Industry participation

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