

Single Catalysts for Reversible Hydrogen Storage and Release “in-from” Methanol Carrier

Context. *SinCare-H2* is a well structured and scientifically challenging project supported by a robust consortium of experimental,⁽¹⁾ catalytic⁽²⁾ and theoretician⁽³⁾ experts in advancing the hydrogen economy.

Our consortium has already demonstrated its ability to work together and showed some proofs of concept in the storage and release processes of dihydrogen, H₂.⁽⁴⁾ *SinCare-H2* project is built to enable innovative and substantial impact on advances in the field of green and sustainable hydrogen energy in the academic discipline and in industry using methanol as a liquid hydrogen carrier.

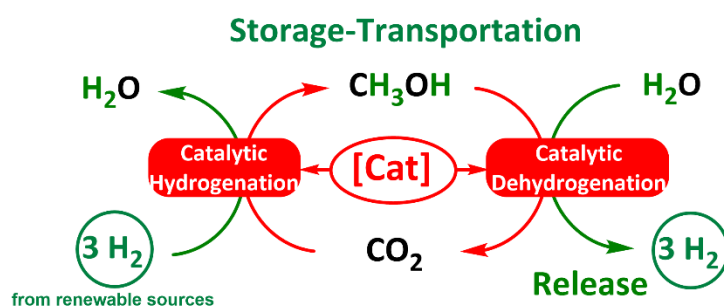
Our 1st generation of dormant active cyclic-one (DAC-Cyclone) complexes demonstrated unprecedented catalytic properties and performances. With a **single catalyst** and **without the addition of any additive**, we are able to store dihydrogen, H₂, in the form of formic acid and release it when the use of dihydrogen is required.⁽⁵⁾

Our unique synthetic pathways offer the opportunity to set up different fine-tuning steps in the preparation of 2nd generation DAC-Cyclone complexes. Our DAC-cyclone catalysts are tunable to a very large extend, there is a multitude of catalysts available.

Objectives. In view of (1) the preliminary results we registered with our unique DAC-Cyclone catalysts and (2) the skills we accumulated these last few years, the design and the chemical reactivity of catalysts able to carry out the storage and release of dihydrogen, H₂, with a single catalyst without any additive are now possible and will be tackle.

The unprecedented concept we developed will be considered with methanol as the liquid organic hydrogen carriers (LOHC) to store dihydrogen, H₂. Methanol has the advantage of containing more hydrogen than formic acid (99 g.L⁻¹ vs 53 g.L⁻¹). The catalytic hydrogenation of CO₂ to MeOH and the reversible catalytic dehydrogenation reaction of MeOH to CO₂ and 3 H₂ are not easy processes and we will tackle these challenges chemical transformations with our 2nd generation DAC-Cyclone catalysts.

SinCare-H2 project is at the interface of organic chemistry, main-group chemistry, coordination chemistry, and homogeneous catalysis for sustainable energy. *SinCare-H2* project will give the post-doctoral fellow the opportunity to benefit and interact with our scientific consortium composed with senior experts in catalysis and theoretical calculations.



Single DAC-Cyclone catalyst, [Cat], for storage-Transportation and release of H₂ using e-MeOH as Green Hydrogen carrier

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(4) J.-M. Sotiropoulos, C. Fischmeister, A. Igau. CatEngy ANR-18-CE07-0006-01

(5) R. Verron, E. Puig, P. Sutra, A. Igau, C. Fischmeister. *Base-Free Reversible Hydrogen Storage Using a Tethered π -Coordinated-Phenoxy Ruthenium-Dimer Precatalyst*. ACS Catalysis **2023**, 13, 5787-5794. E. Puig, R. Veron, M. Kechaou-Perrot, L. Vendier, H. Gornitzka, K. Miqueu, J.-M. Sotiropoulos, C. Fischmeister, P. Sutra, A. Igau, *Shvo-type metal–ligand cooperative catalysts: tethered η^5 -oxocyclohexadienyl ruthenium complexes*. Organometallics **2022**, 41, 1391-1402.

Candidate Profile. We are looking for a highly motivated post-doctorate fellow. Previous experience relying with the preparation of ruthenium and/or iron transition metal complexes is a prerequisite in this collaborative research project. Precision and rigor will be necessary to develop this project.

Starting date. September-October 2025. **Duration.** one year (+ one year).

Language. English

Founding ANR *SinCare-H2* project CNRS as employer.

Application procedure: By e-mail only (alain.igau@lcc-toulouse.fr) with the subject of the message “Post-Doc Application to ANR-SinCare-H2” including a CV, list of publications, and 2 senior researchers referees.