Statistical learning for converging strategies in thermal and electrochemical conversion of small molecules

Timeline | 04/2021 to 02/20224

ICIQ People | Nuria López Research Group

Budget | 160.000 CHF

Call | NCCR Catalysis

SUMMARY

The conversion of small molecules to useful chemicals like fuels and commodities could benefit our benefit our society by reducing the (i) most abundant climate change generator closing the carbon cycle and if coupled to renewable energy sources (ii) reduce the energy demand for the activation of such inert molecule.1Most of the active catalytic materials to activate small molecules (i.e. CO_2) contain oxides and metals in variable combinations but: (i) the chemical nature of the individual catalytic parts (metallic and a polarized) is difficult to identify experimentally; (ii) the synergies between them as they form complex interfaces have prevented a rational design of new catalysts based on atomistic principles; and (iii) general activity equations for rates and selectivity are missing. Our goal is to rationalize the series of metals, oxides and their combinations to provide a robust framework that can identify interfaces both for the thermal and electrochemical. To this end, starting by the traditional Density Functional Theory methodologies a series of Statistical Learning (SL) and artificial intelligence techniques including, but not limited to, dimensionality reduction; Bayesian inference and neural networks will be employed.

FNSNF Swiss National Science Foundation

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