# Computational materials science towards environmentally friendly materials

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The science world is evolving towards the design of cost-effective, environmental friendly, and efficient materials for the development of renewable energy technologies. The supercomputers and computational chemistry are essential tools to speed up the study of materials properties for industrial proposes. In this talk, I will present two examples in two different research fields (heterogeneous catalysis and Li-ion batteries) to show the importance and the utility of computational calculations to improve the materials design processes.

First of all, $CO_2$ activation and conversion towards valuable added compounds is a major scientific challenge. Sophisticated experiments and calculations based on periodic density functional theory were used to study the unique behavior of molybdenum carbide surfaces and of Cu clusters supported thereon to provide the evidence of the impact of the metal/carbon ratio in the carbide, essential for the design of new active catalysts.

In the field of Li-ion batteries, to switch the organic liquid electrolytes is a chief challenge due to the electrolyte's flammability, cost and toxicity. The substitution of organic electrolytes by aqueous solutions is a hot topic although the interaction of the electrodes with water leads to many detrimental mechanisms that are currently often hypothesized but not very well explored. I will present the analysis of the proton insertion mechanism by means of computations, in order to investigate the detrimental phenomena in cathode materials.