

Simulations in electrocatalytic reduction of CO₂

Nuria Lopez

Institute of Chemical Research of Catalonia, Av. Països Catalans 16, 43007 Tarragona, Spain

CO₂ reduction with renewable energies opens the path to close the carbon cycle. Simulations have provided relevant insight on some important aspects of the materials under true reaction conditions. The materials under reaction conditions reconstruct and rearrange very extensively, these can be understood via the simulations as the direct observation is sometimes extremely challenging. Moreover, the electrolyte contributes to the overall activity and selectivity but the intimate mechanisms are still under debate. Finally, in many cases the activity towards compounds with more than two carbon atoms is limited to the use of copper. However, over the last years we have devised alternative materials that can break the copper limits.