
Designing Active Materials toward Formic Acid Reduction

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Language Undefined

Description:

Proyecto asignado a través de la [Red Española de Supercomputación](#) [2].

The electrochemical reduction of formic acid (FAR) is still an unsolved challenge in CO₂ transformation into commodities and fuels with high energy densities. Indeed, previous experimental results have shown that several materials reduce CO₂ only to formic acid. In this work, using DFT calculations, we will model all the different mechanistic possibilities on several metals and oxides to unravel the special characteristics that efficient FAR catalysts should have. Based on those, we will design and test new materials for FAR to methanol.

Source URL:<https://web.computaex.es/en/proyectos/designing-active-materials-toward-formic-acid-reduction>

Links

[1] <https://www.ub.edu/> [2] <https://www.res.es/>