Origin of the selectivity on the conversion of CO2 on ceria supported Ni catalyst from multiscale simulations

Investigadores:

- Francesc Illas. Faculty of Chemistry, University of Barcelona (UB [1]).

Idioma Sin definir

Descripción:

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

Conversion of atmospheric CO_2 is a need to prevent further global warming and also constitutes an opportunity as it can be used as a C1 feedstock for the synthesis of fuels and other commodities. However, the high stability of this molecule requires high active catalysts, often transition metals, leading to a mixture of products. Here, the selectivity of Ni on a ceria support towards CO_2 conversion will be studied by multiscale modelling simulations and compared to that of previous studies for extended Ni surfaces and Ni nanoparticles supported on TiC. This will provide useful information for the development of more efficient and selective catalyst.

URL del envío:https://www.cenits.es/proyectos/origin-selectivity-conversion-co2-ceria-supported-ni-catalyst-multiscale-simulations

Enlaces

[1] https://www.ub.edu/web/portal/ca/ [2] https://www.res.es/