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43GERSEQ
Ciudad Real 2023

Graphite-encapsulated iron nanoparticles: an evaluation of their use as a catalyst for the production of energy and high value-added products.

Gisele Giovanna Halfeld
Víctor J. Climent Payá
Natalia García Rey

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  - Fuel cells
  - Catalysts
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  - Graphite encapsulated iron nanoparticles
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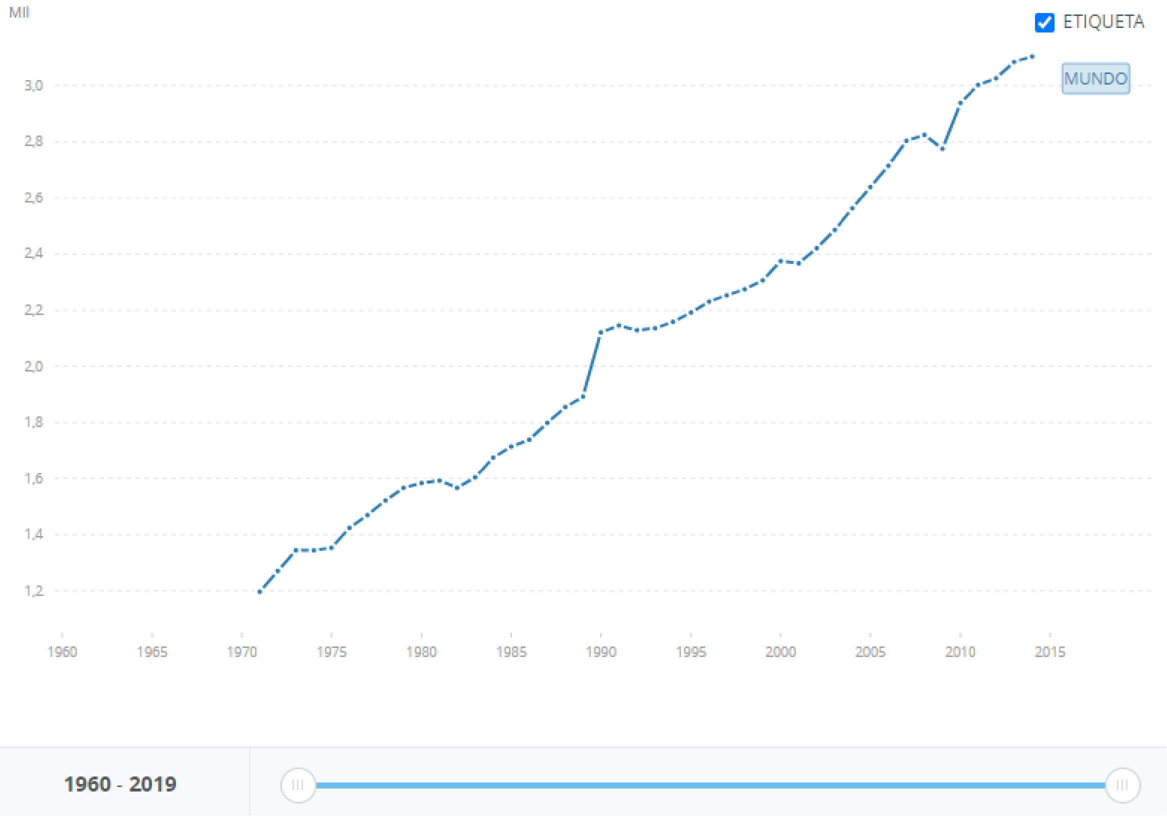
Electrical energy consumption (kWh per capita)



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Agencia Internacional de la Energía (AIE) (Estadísticas de la AIE © OCDE/AIE, iea.org/stats/index.asp); Estadísticas de energía y balances de países no pertenecientes a la OCDE; Estadísticas de energía de países de la OCDE, y balances de energía de países de la OCDE.

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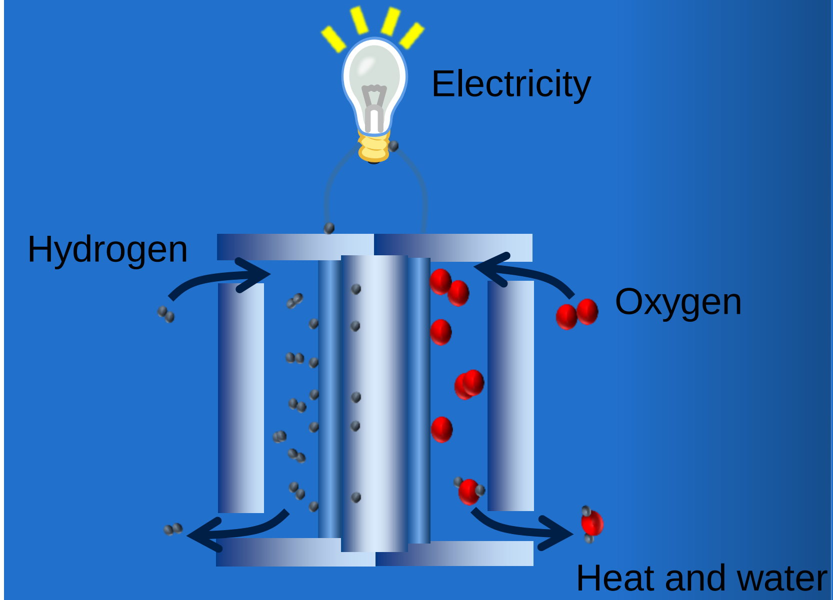
Green H2 to power the world

Transform chemical energy into electrical energy

High efficiency

High cost of production

Low environmental impact



CHANDRAN, Priji; GHOSH, Arpita; RAMAPRABHU, Sundara. High-performance Platinum-free oxygen reduction reaction and hydrogen oxidation reaction catalyst in polymer electrolyte membrane fuel cell. Scientific reports, v. 8, n. 1, p. 3591, 2018.

Catalysts

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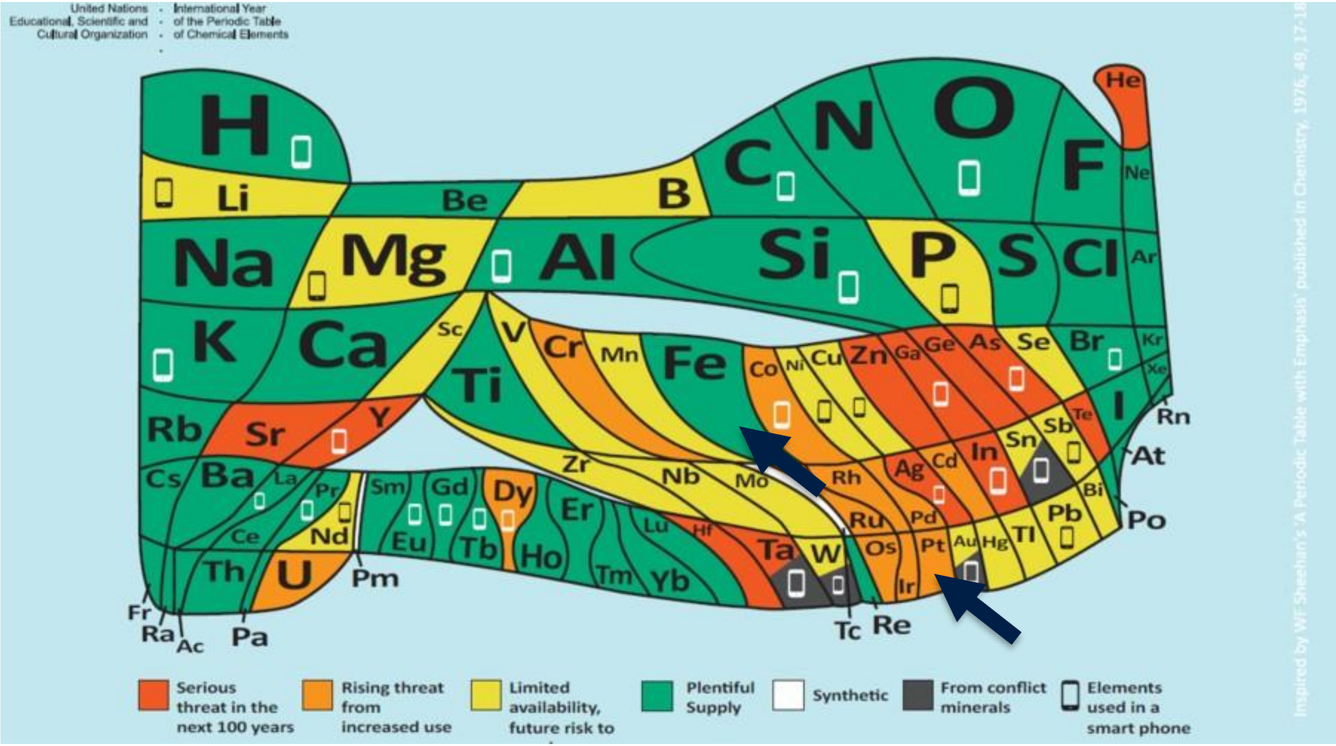


"If all of the remaining lithospheric stock of platinum were dedicated to operating a fleet of 500 million fuel cell vehicles, the platinum resource in the lithosphere could sustain this fleet for 15 years."

(R.B. Gordon et al, PNAS 103 (2006) 1209 DOI: 10.1073/pnas.0509498103)

Iron nanoparticles

ELSEVIER

Contents lists available at ScienceDirect

Nano Energy

journal homepage: www.elsevier.com/locate/nanoen

One-step conversion from Ni/Fe polyphthalocyanine to N-doped carbon supported Ni-Fe nanoparticles for highly efficient water splitting

Zhengping Zhang, Yeshen Qin, Meiling Dou, Jing Ji, Feng Wang*

State Key Laboratory of Chemical Resource Engineering, Beijing Key Laboratory of Electrochemical Process and Technology for Materials, Beijing University of Chemical Technology, Beijing 100029, China

ZHANG, Zhengping et al. One-step conversion from Ni/Fe polyphthalocyanine to N-doped carbon supported Ni-Fe nanoparticles for highly efficient water splitting. Nano Energy, v. 30, p. 426-433, 2016.

Iron nanoparticles

Contents lists available at ScienceDirect

Electrochimica Acta

journal homepage: www.elsevier.com/locate/electacta

ELSEVIER

Carbon-encapsulated nickel-iron nanoparticles supported on nickel foam as a catalyst electrode for urea electrolysis

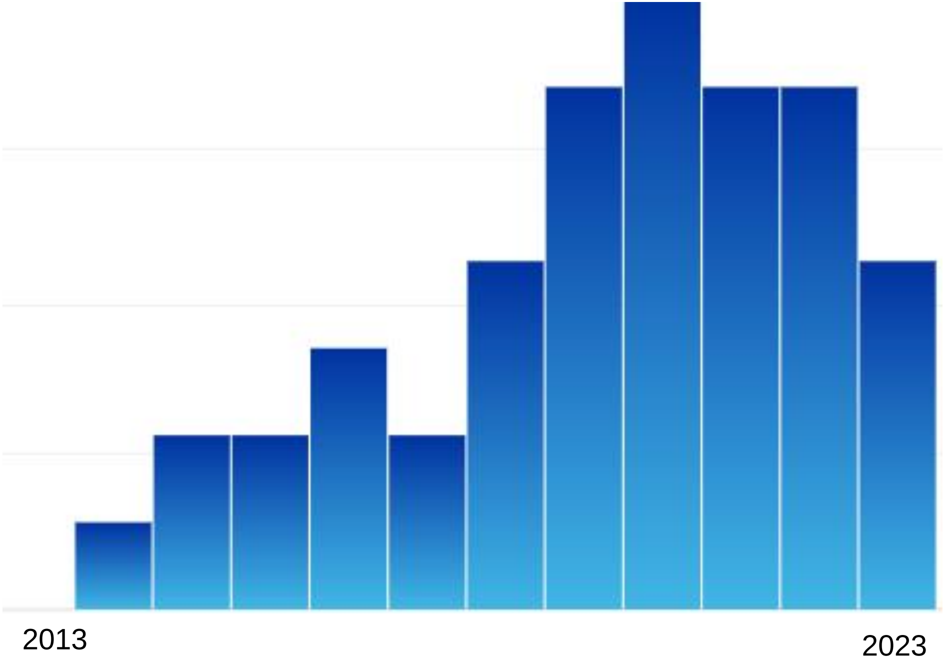
Mao-Sung Wu*, Chi-Yu Jao, Farn-Yih Chuang, Fang-Yi Chen

Department of Chemical and Materials Engineering, National Kaohsiung University of Applied Sciences, Kaohsiung 807, Taiwan

WU, Mao-Sung et al. Carbon-encapsulated nickel-iron nanoparticles supported on nickel foam as a catalyst electrode for urea electrolysis. Electrochimica Acta, v. 227, p. 210-216, 2017.

Iron nanoparticles

Number of publications on the use of nanoparticles with iron as a catalyst for the evolution of hydrogen: 43



Fonte: Sci-finder Junho- 2023

Iron nanoparticles

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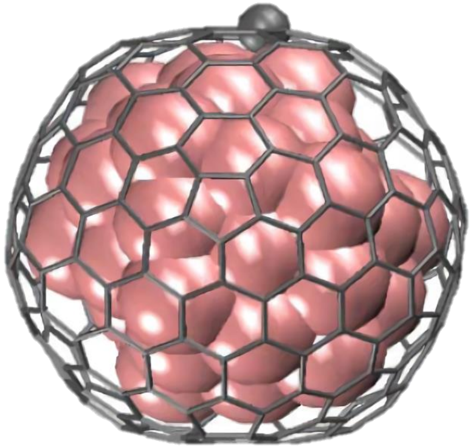
TAVAKKOLI, Mohammad et al. Single-shell carbon-encapsulated iron nanoparticles: synthesis and high electrocatalytic activity for hydrogen evolution reaction. Angewandte Chemie International Edition, v. 54, n. 15, p. 4535-4538, 2015.

CILPA-KARHU, Geraldine; PAKKANEN, Olli J.; LAASONEN, Kari. Hydrogen evolution reaction on the single-shell carbon-encapsulated iron nanoparticle: a density functional theory insight. The Journal of Physical Chemistry C, v. 123, n. 22, p. 13569-13577, 2019.

VARNELL, Jason A. et al. Identification of carbon-encapsulated iron nanoparticles as active species in non-precious metal oxygen reduction catalysts. Nature communications, v. 7, n. 1, p. 12582, 2016.

Carbon-encapsulated iron nanoparticles

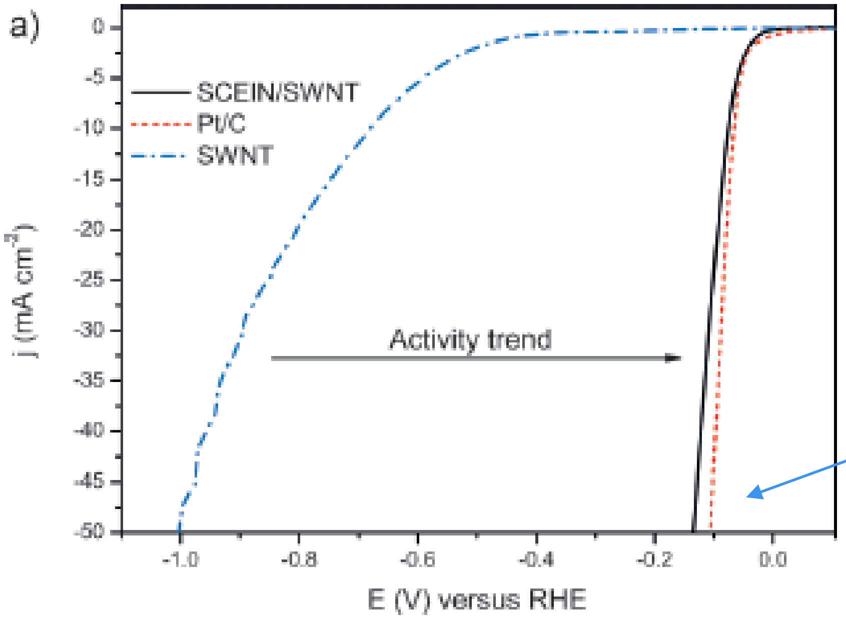
Increase stability of nZVI



CILPA-KARHU, Geraldine; PAKKANEN, Olli J.; LAASONEN, Kari. Hydrogen evolution reaction on the single-shell carbon-encapsulated iron nanoparticle: a density functional theory insight. The Journal of Physical Chemistry C, v. 123, n. 22, p. 13569-13577, 2019.

Catalysts

Polarization curve



SCEINs single layer carbon encapsulated iron nanoparticles

Pt/C commercial Pt catalyst (20%)

SWNTs single wall carbon nanotubes

slightly negative voltage to overcome the activation energy

CILPA-KARHU, Geraldine; PAKKANEN, Olli J.; LAASONEN, Kari. Hydrogen evolution reaction on the single-shell carbon-encapsulated iron nanoparticle: a density functional theory insight. The Journal of Physical Chemistry C, v. 123, n. 22, p. 13569-13577, 2019.

Graphite encapsulated iron nanoparticles

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E4CE
ENGINEERING FOR CIRCULAR ECONOMY

Calpech

ACS Sustainable Chemistry & Engineering
Research Article
Cite This: ACS Sustainable Chem. Eng. 2018, 6, 7995–8002
pubs.acs.org/journal/ascecg

Green Synthesis of Thin Shell Carbon-Encapsulated Iron Nanoparticles via Hydrothermal Carbonization

B. Calderon,* F. Smith, I. Aracil, and A. Fullana

Chemical Engineering Department, University of Alicante, San Vicente del Raspeig Road, s/n 03690 San Vicente del Raspeig, Alicante, Spain

Encapsulation of nZVI within micro or nano carbon spheres through hydrothermal carbonization (HTC)

CALDERON, Blanca et al. Green synthesis of thin shell carbon-encapsulated iron nanoparticles via hydrothermal carbonization. ACS Sustainable Chemistry & Engineering, v. 6, n. 6, p. 7995-8002, 2018.

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- Elimination of hydrogen sulfide in biodigesters
- Improvement of biogas production
- Elimination of heavy metals in contaminated water and soil
- Desulfurization of gas streams
- Denitrification of aquifers

CALDERON, Blanca et al. Green synthesis of thin shell carbon-encapsulated iron nanoparticles via hydrothermal carbonization. ACS Sustainable Chemistry & Engineering, v. 6, n. 6, p. 7995-8002, 2018.

Synthesis CE-nFe

0.057 mole de $Fe(NO3)3\cdot 9H2O$ + 300 mL olive mill wastewater (1H)

Hydrothermal reactor at 200ºC for 3H

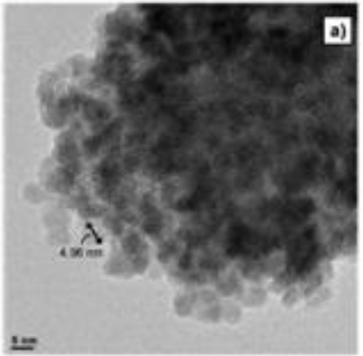
Vacuum filtered with cellulose acetate 0,2 μm

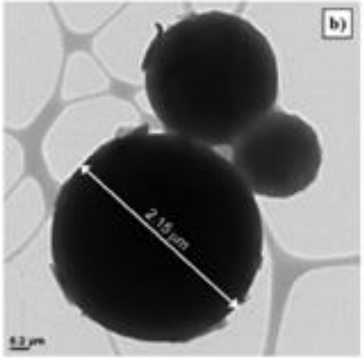
Wash twice with an ethanol-water solution 50/50 (v/v).

Dried at 80 °C for 12 h

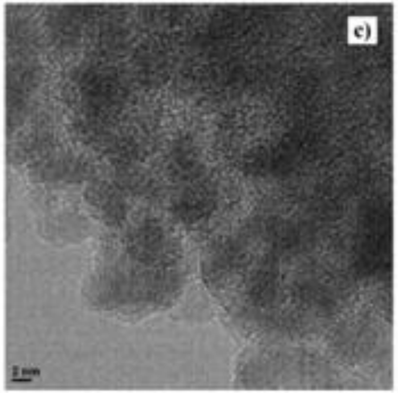
CALDERON, Blanca et al. Green synthesis of thin shell carbon-encapsulated iron nanoparticles via hydrothermal carbonization. ACS Sustainable Chemistry & Engineering, v. 6, n. 6, p. 7995-8002, 2018.

OMW-CE-nFe (5 nm)





G-CE-nFe 0.2 (μm)



The smaller size and more porous structure of OMW-CE-nFe provide the material with a higher surface area

G-CE-nFe consisted of microspheres of diameters of 2.0 ± 0.7 μm, OMW-CE-nFe presented a sphere-like nanostructure of sizes of 130 ± 50 nm

Figure. TEM images of (a) OMW-CE-nFe (b) G-CEnFe (c) HRTEM image of the nanoparticles shell of OMW-CE-nFe

CALDERON, Blanca et al. Green synthesis of thin shell carbon-encapsulated iron nanoparticles via hydrothermal carbonization. ACS Sustainable Chemistry & Engineering, v. 6, n. 6, p. 7995-8002, 2018.

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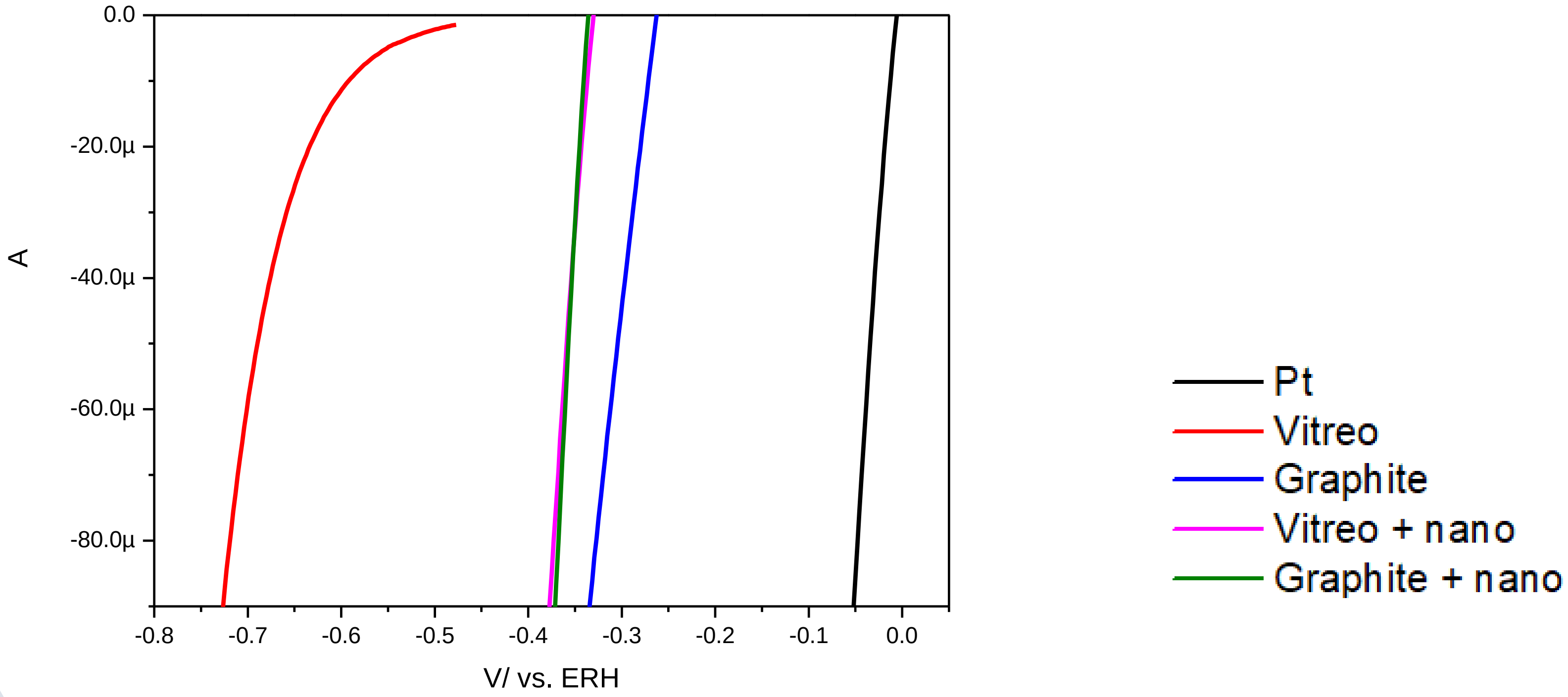
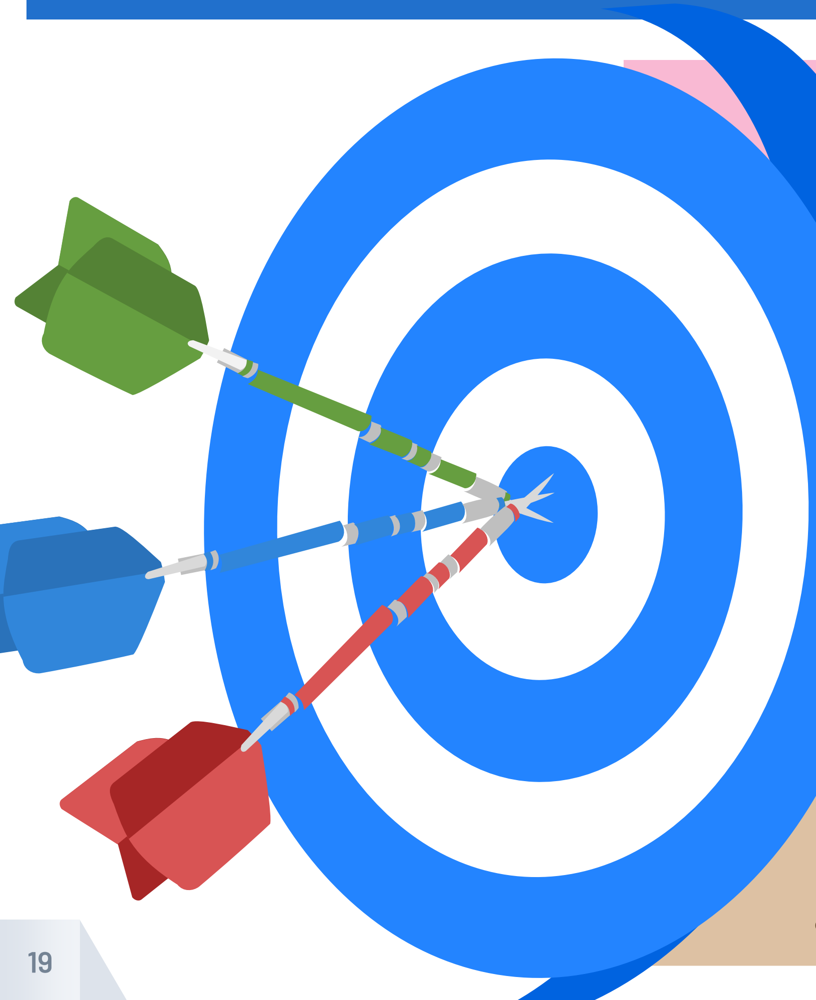
Goal

Test to evaluate the response of nanoparticles the way we received them.





Study the catalysis of various reactions of technological interest

Investigate the interfacial properties in order to establish correlations with their catalytic activity.

Search for the descriptors that characterize the best catalytic activity

Investigate and better understand the mechanisms involved in catalytic activity.

Improve the process of synthesis, purification and post-treatment (maximum activity).

Methodology

Pre treatment:

Composition of the electrolyte, pH, synthesis, concentration, nanoparticle preparation, centrifugation, magnetic sepation, electrophoresis, selective oxidation, oxidarion with nitric acid, doped with nitrogen and phosphorus.

Physical chemical characterization:

FTIR, Raman, DEMS, XPS, SEM, HRTEM

Reactivity:

Cyclic voltammetry and chronoamperometry, impedance spectroscopy, laser-induced temperature jump technique,

Temporary planning

01

2023

Bibliographic search, initial essays with the sample "as it is received". The methods, the characterization techniques will be optimized.

23/24

02

Test different methods of purification. Hydrogen evolution test with the different purified samples.

03

2024

Test with activation methods. Test of hydrogen evolution and oxygen reduction with activated samples.

2025

04

CO_2 reduction and NH_3 oxidation assay. Writing of the thesis.

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Expected impact

Alternative to the use of platinum electrodes

Economical, abundant and easily scalable.

Sustainable energy model based on hydrogen

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Thank you!