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SANTANDER 2022

Estudios Fundamentales y Electrocatálisis en Superficies Bimetálicas Monocristalinas De PtPd

Fundamental Studies and Electrocatalysis on Monocrystalline Bimetallic Surfaces of PtPd

Candidato: Gabriel Melle*

Mentor: Enrique Herrero
Director: Rosa M. Arán-Ais

Santander, 6 - 8 de Julio de 2022

AGENDA

1. **ANTECEDENTES Y ESTADO ACTUAL DEL TEMA**
2. **OBJETIVOS DE LA INVESTIGACIÓN**
3. **METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL**
4. **IMPACTO ESPERADO**

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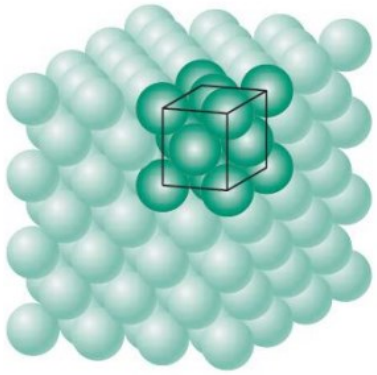
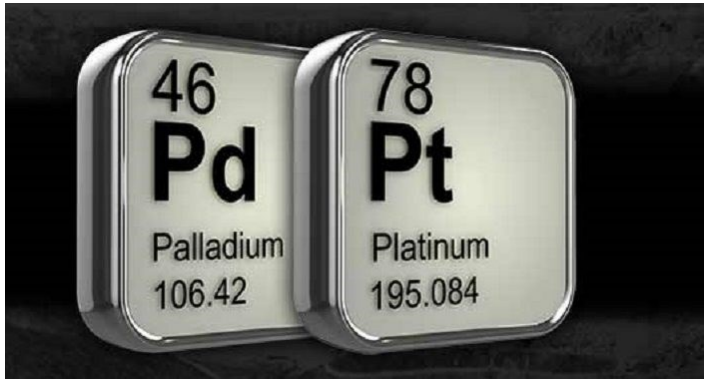
4. **IMPACTO ESPERADO**
5. **RESULTADOS INICIAIS** 

ANTECEDENTES Y ESTADO ACTUAL DEL TEMA

PLATINUM AND PALLADIUM: BROTHER ELEMENTS



Face-Centered Cubic



Lanthanide contraction

ANTECEDENTES Y ESTADO ACTUAL DEL TEMA

PLATINUM AND PALLADIUM AMONG THE BEST CATALYSTS FOR OXIDATION OF ORGANIC MOLECULES.

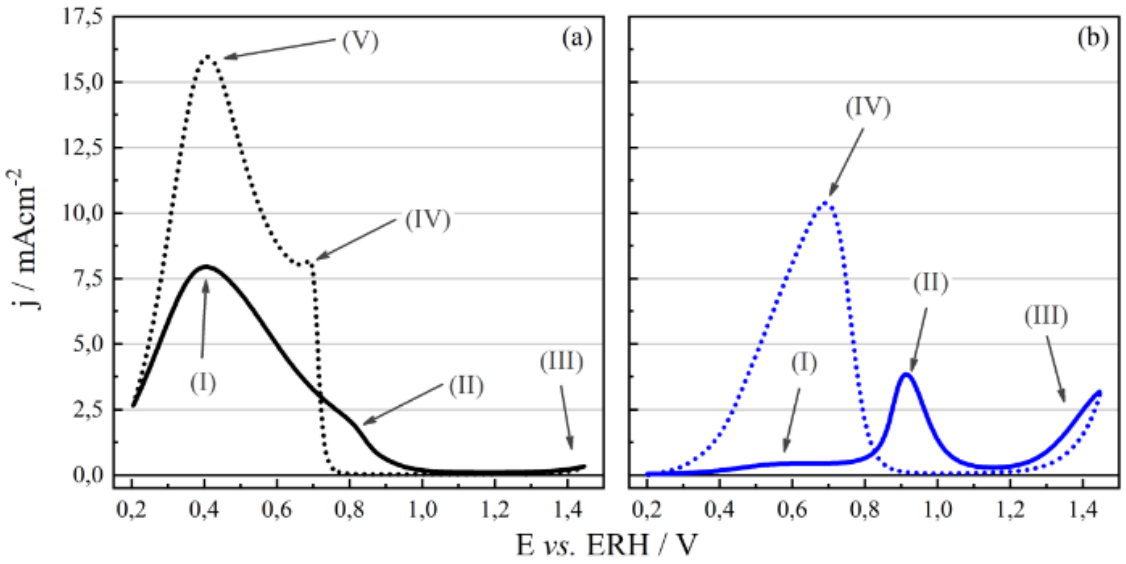


Fig. 1 –Cyclic voltammogram of the electro-oxidation of formic acid in (a) Pd or (b) Pt in acidic medium. figure adapted from reference [2]

Trial and Error

Designed Search

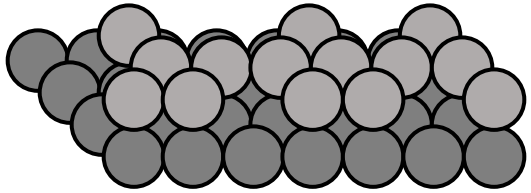
[1] Parsons, R.; Vandernoot, T.J. Electroanal. Chem.1988,257,9−45.
[2] Melle, G, Romano, R., Altair, T., & Varela, H. (2020, November). *ECS Meeting Abstracts* (No. 68, p. 3676). IOP Publishing

ANTECEDENTES Y ESTADO ACTUAL DEL TEMA

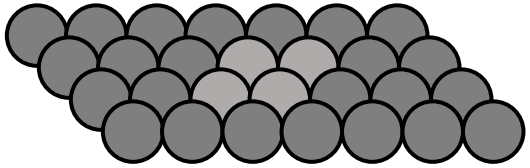
Palladium Electrodeposition on Pt single Crystal

VS.

Pt–Pd single Crystal bimetallic



model surface



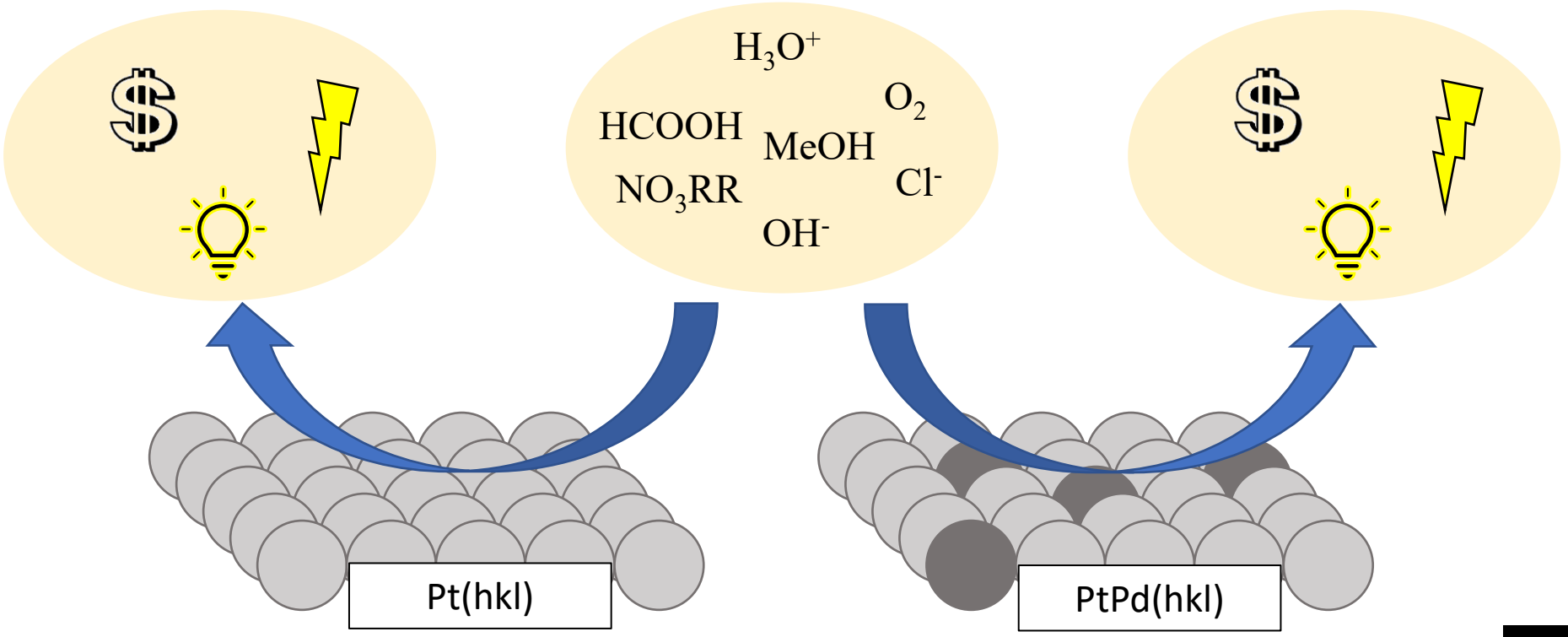
Well-defined
model surface

Palladium

Platinum

Objetivos de La Investigación

To carry out a fundamental study of the electrochemical behaviour of PtPd bimetallic electrodes as well as to investigate its catalytic activity in reactions with potential use in energy generation.



METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL

CONFECTION AND CHARACTERIZATION OF THE ELECTRODES

CATALYTIC ACTIVITY OF THE ELECTRODES

[1] Clavilier, J. et all, Journal of Electroanalytical Chemistry and Interfacial Electrochemistry 107, 205–209 (1980).

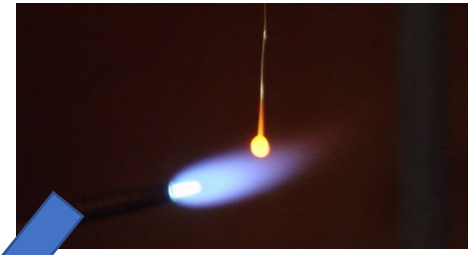
METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL

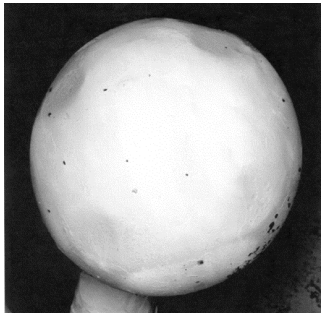
Activated	Semester					
	I	II	III	IV	V	VI

METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL

CONFECTION AND CHARACTERIZATION OF THE ELECTRODES:

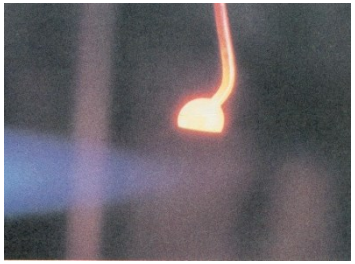
- Confection by protocol developed by Clavilier [1]
- Physical Characteristics
- Electrochemical Characteristics

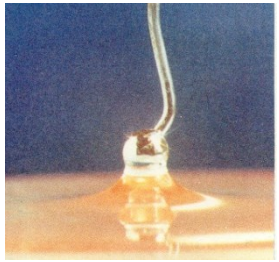




CATALYTIC ACTIVITY OF THE ELECTRODES:

- **L**ow **E**nergy **E**lectron **D**iffraction (LEED)
- **X**-ray **P**hotoelectron **S**pectroscopy (XPS)
- **V**oltammogram **P**rofile





[1] Clavilier, J. et all, Journal of Electroanalytical Chemistry and Interfacial Electrochemistry 107, 205–209 (1980).

METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL

CONFECTION AND CHARACTERIZATION OF THE ELECTRODES:

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CATALYTIC ACTIVITY OF THE ELECTRODES:

- Formic Acid oxidation reaction (FAOR)
- Methanol and Ethanol Oxidation on Alkaline Medium
- Nitrate reduction reactions (NO_3RR)
- anything else?

METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL

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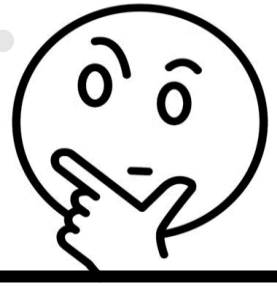
CATALYTIC ACTIVITY OF THE ELECTRODES:

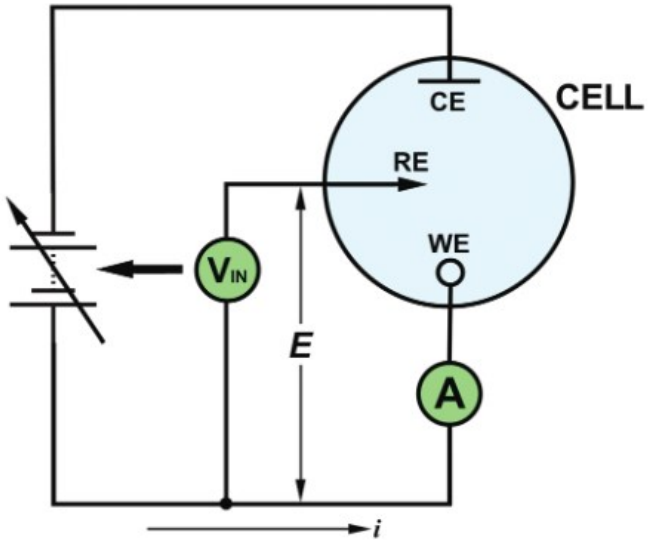
- Formic Acid oxidation reaction (FAOR)
- Methanol and Ethanol Oxidation on Alkaline Medium
- Nitrate reduction reactions (NO_3RR)
- anything else?

Which one is the best?
X
Why is this better?



METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL

- **Experimental setup and methodology**



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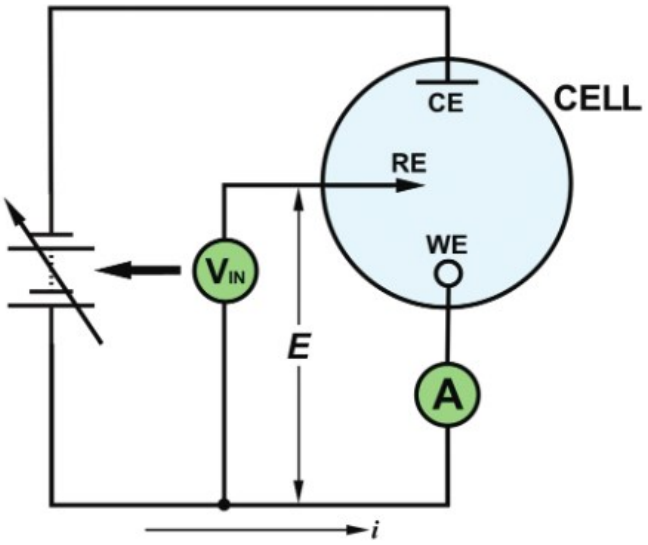
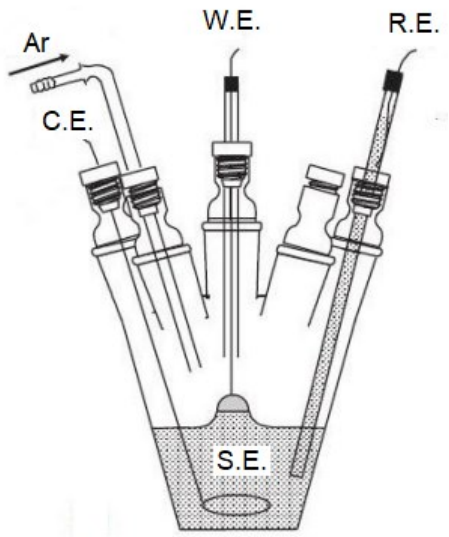


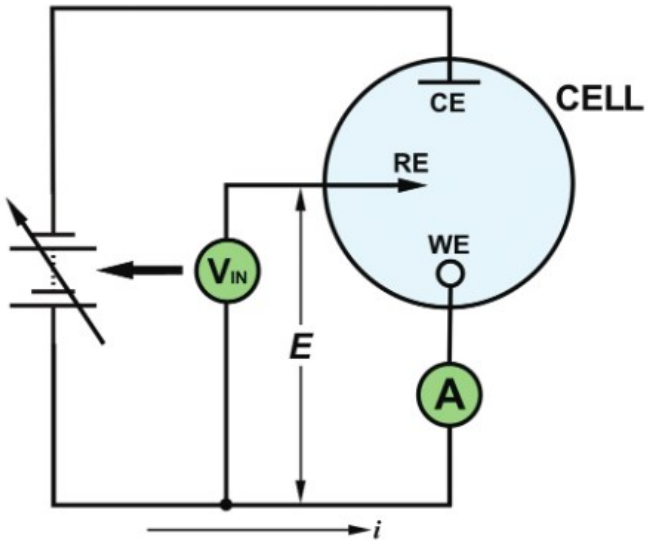


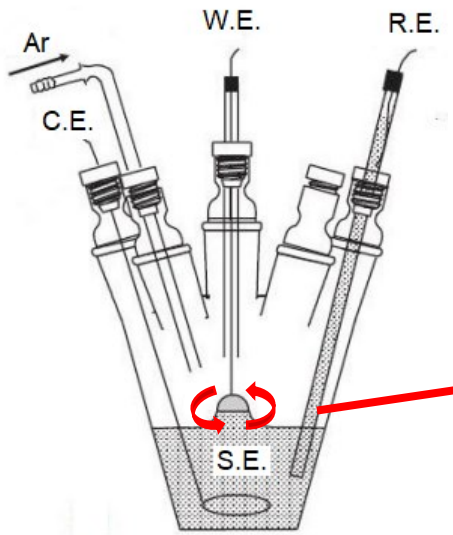
Voltammetry

- Classic
- High-Scan-Rate
- Pulsed

METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL

- **Experimental setup and methodology**





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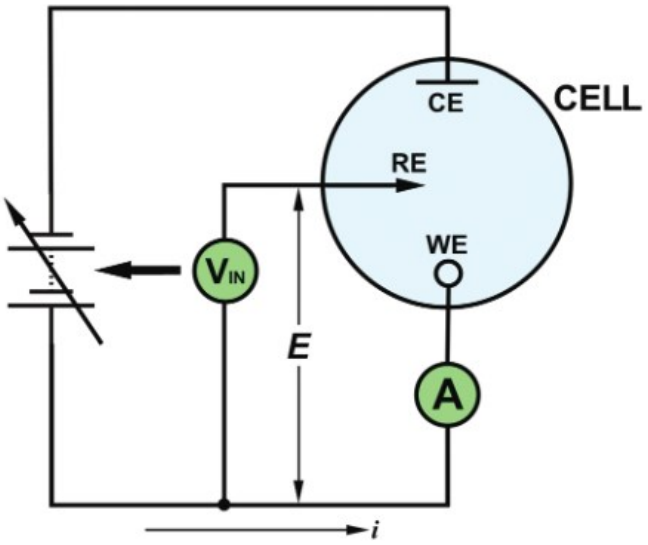
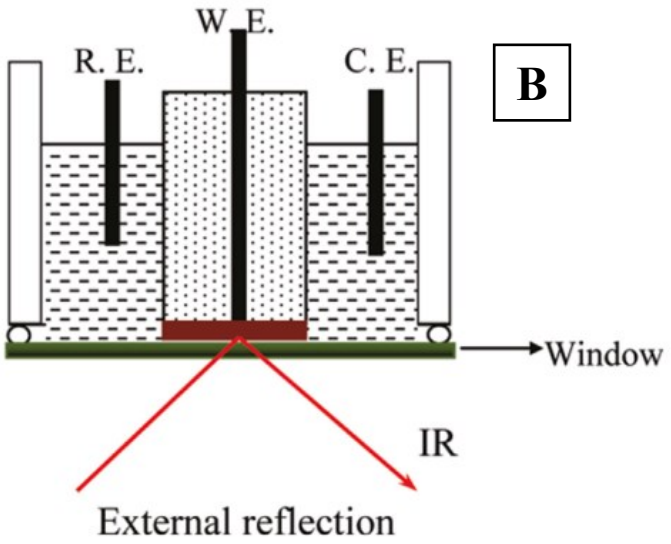
Colburn, Alex W., et al. Physical Chemistry Chemical Physics 23.14 (2021): 8100-8117.

METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL

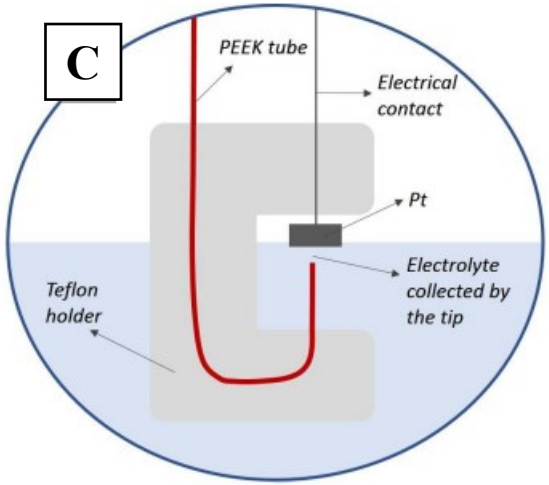
- **Experimental setup and methodology**





Ye, Jin-Yu, et al. *Nano Energy* 29 (2016): 414-427.

Voltammetry combined with FTIR, DEMS and HPLC



Melle, Gabriel, et al. *Electrochimica Acta* 398 (2021): 139318.

Colburn, Alex W., et al. Physical Chemistry Chemical Physics 23.14 (2021): 8100-8117.

METODOLOGÍA, HIPÓTESIS Y PLANIFICACIÓN TEMPORAL

- **Experimental setup and methodology**

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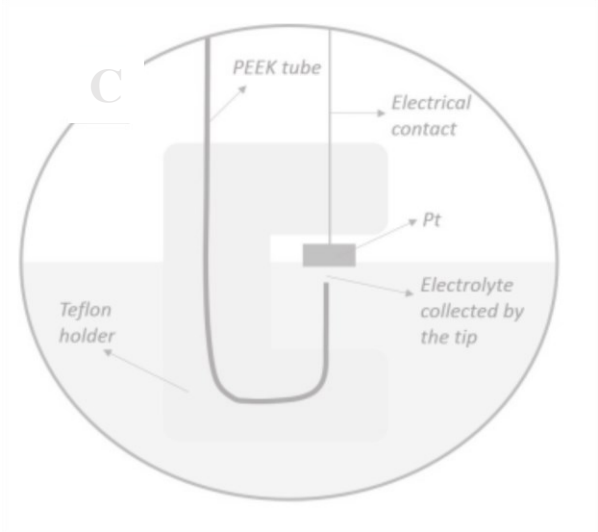
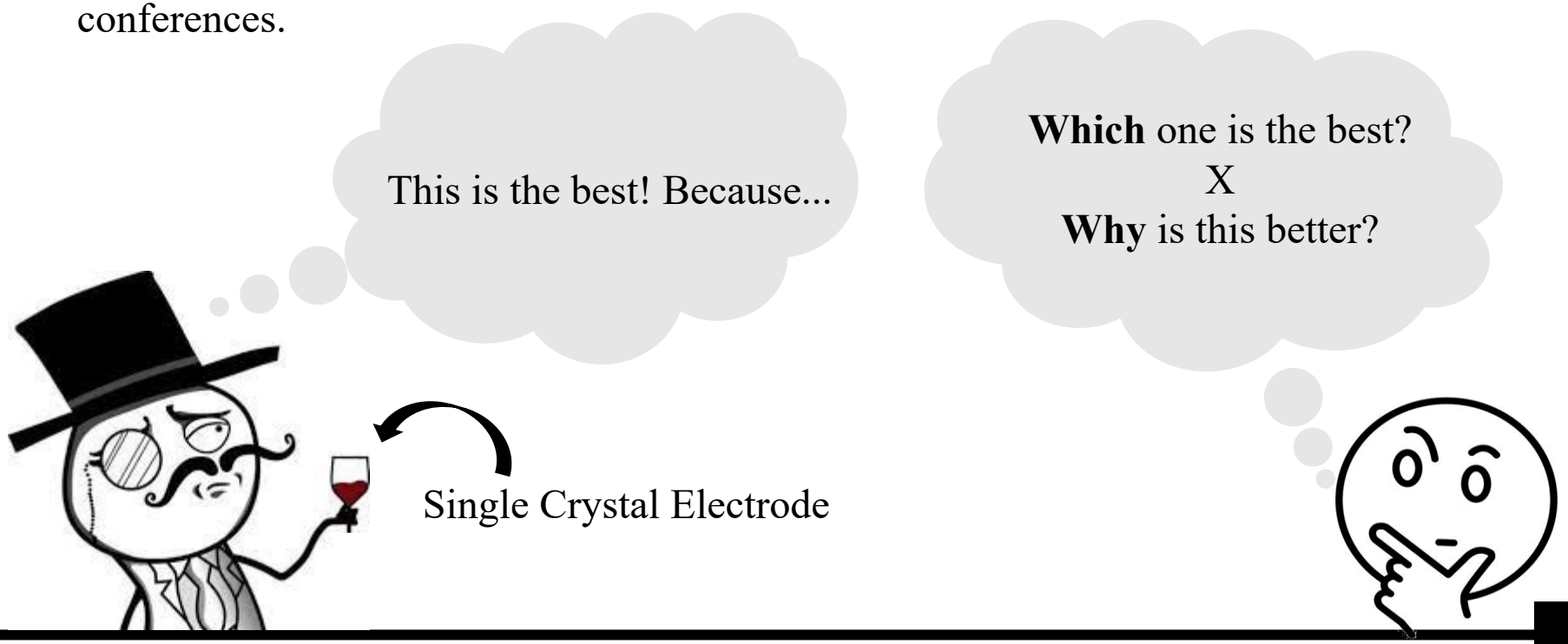


Melle, Gabriel,

- **Mathematical model and numerical simulation**

IMPACTO ESPERADO

- That the student has acquired high knowledge in electrochemistry, as well as in solving complex scientific problems;
- Publication of results in scientific journals;
- Presentation by the student of the results obtained by the scientific community through conferences.



INITIAL RESULTS

INITIAL RESULTS - Characterization of electrodes.

Low **E**nergy **E**lectron **D**iffraction (LEED) and **X**-ray **P**hotoelectron **S**pectroscopy (XPS).

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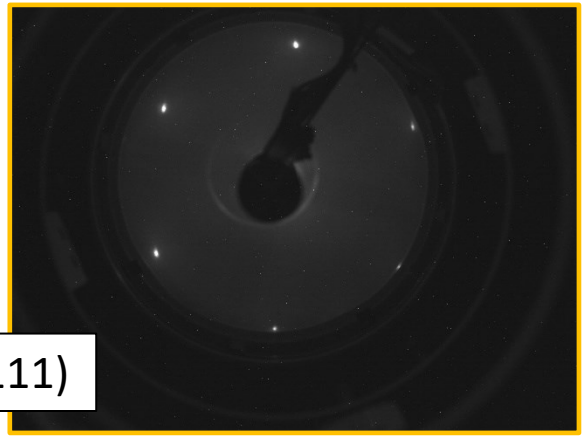
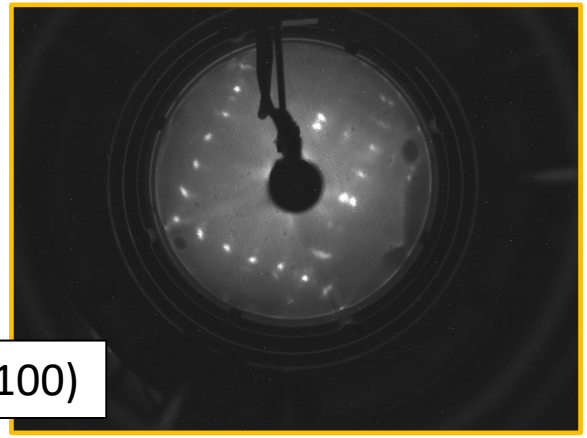


$Pt_{90}Pd_{10}(111)$



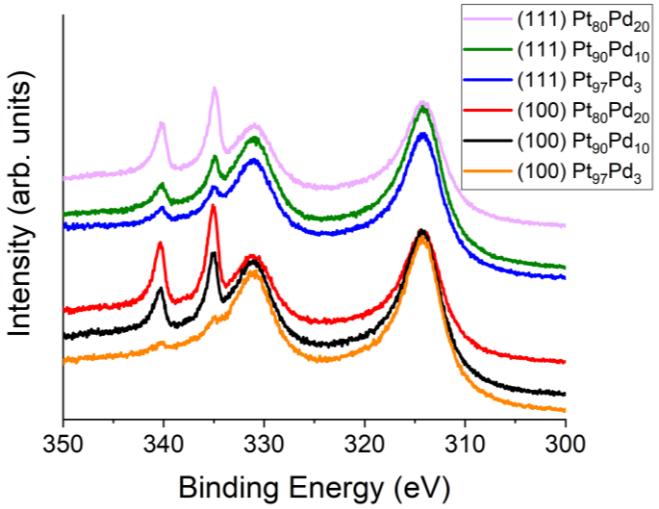
$Pt_{90}Pd_{10}(100)$

INITIAL RESULTS - Characterization of electrodes.

Low Energy Electron Diffraction (LEED) and **X**-ray **P**hotoelectron **S**pectroscopy (XPS).

$Pt_{90}Pd_{10}(111)$

$Pt_{90}Pd_{10}(100)$



Sample (nominal Ratio)	XPS – Integrated Area
$Pt_{80}Pd_{20}$ (100)	85 % (Pt) - 15 % (Pd)
$Pt_{90}Pd_{10}$ (100)	93 % (Pt) - 7 % (Pd)
$Pt_{97}Pd_{3}$ (100)	99 % (Pt) - 1 % (Pd)
$Pt_{80}Pd_{20}$ (111)	88 % (Pt) - 12 % (Pd)
$Pt_{90}Pd_{10}$ (111)	96 % (Pt) - 4 % (Pd)
$Pt_{97}Pd_{3}$ (111)	97 % (Pt) - 3 % (Pd)

INITIAL RESULTS - Characterization of electrodes.

PtPd(111) - Cyclic Voltammetric (CV)

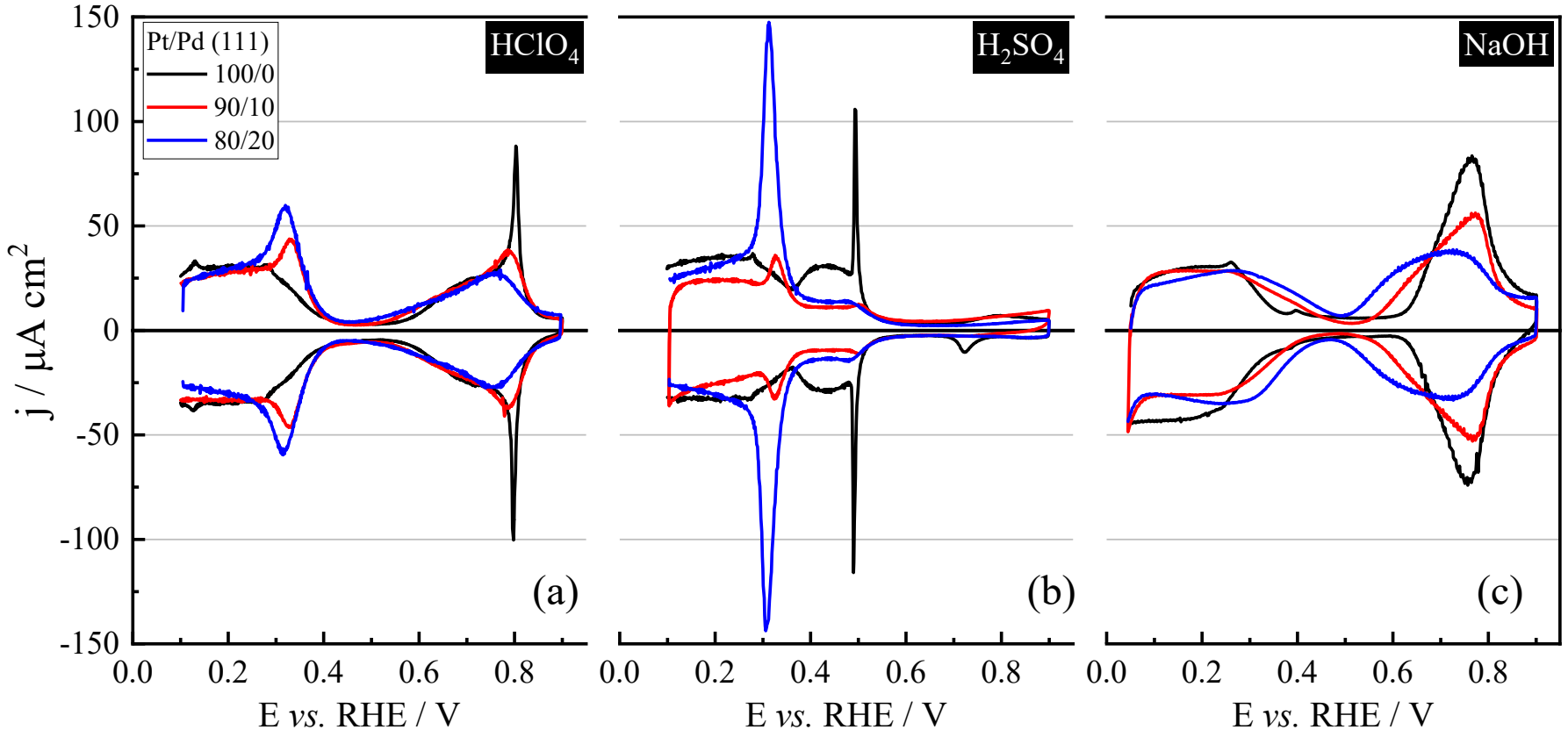


Fig. 2 - Voltammetric profile of the electrodes of the family (111) , obtained at 0.05 V s^{-1} in 0.1 M (a) $HClO_4$, (b) H_2SO_4 or (c) NaOH.

INITIAL RESULTS - Characterization of electrodes.

PtPd(111) – Formic **A**cid **E**lectro-**O**xidaction **R**eaction (FAEOR)

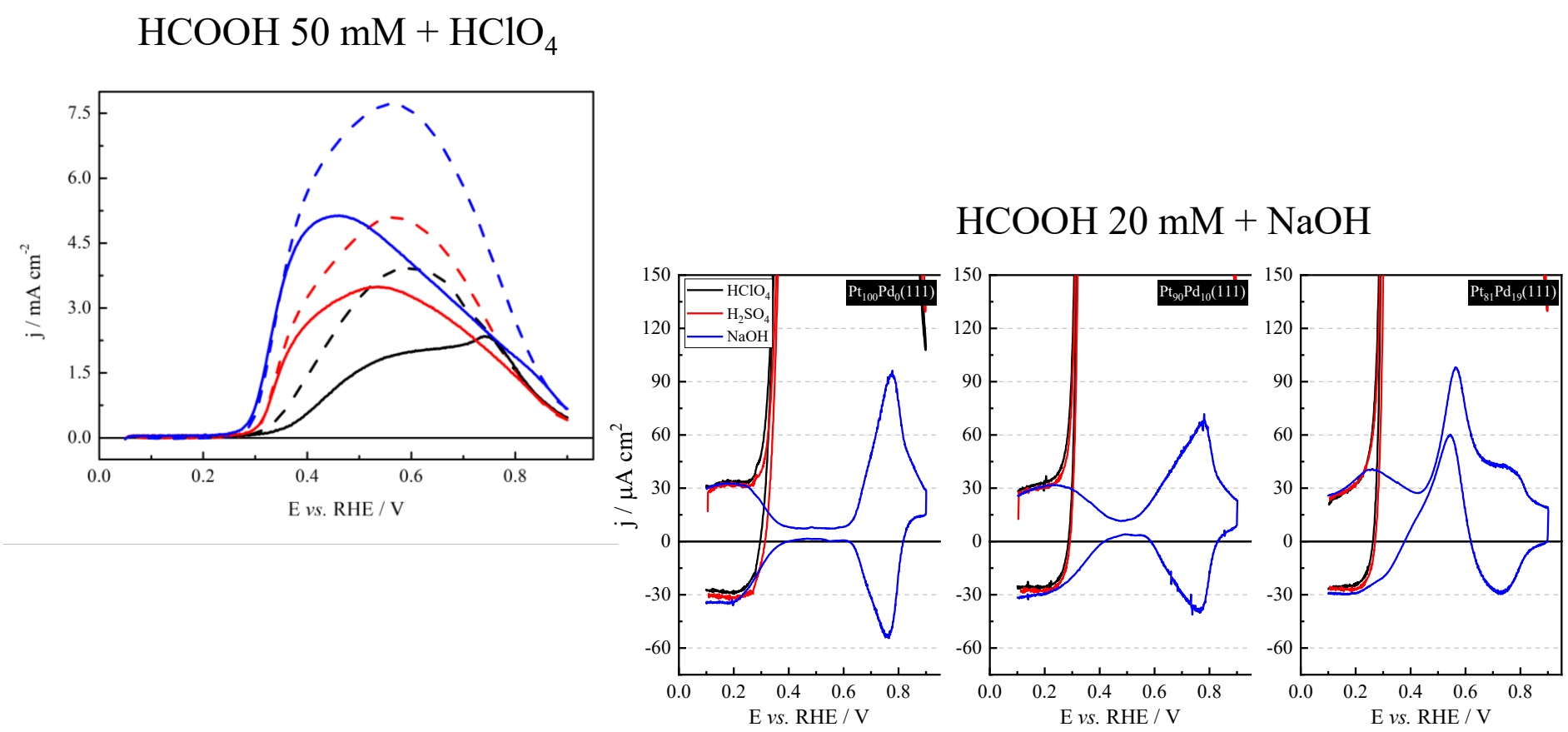


Fig. 3 – FAEOR on Pt(111) or PtPd(111) Family in acid or alcaline medio. Solid and dotted lines represent positive and negative going scans, respectively. $|dE/dt| = 0.05$ V s^{-1}; $[HClO_4]$ and $[NaOH] = 0.1$ mol L^{-1}.

INITIAL RESULTS - Characterization of electrodes.

PtPd(111) x PtPd(100) – Formic **A**cid **E**lectro-**O**xidaction **R**eaction (FAEOR)

PtPd(111) **PtPd(100)**

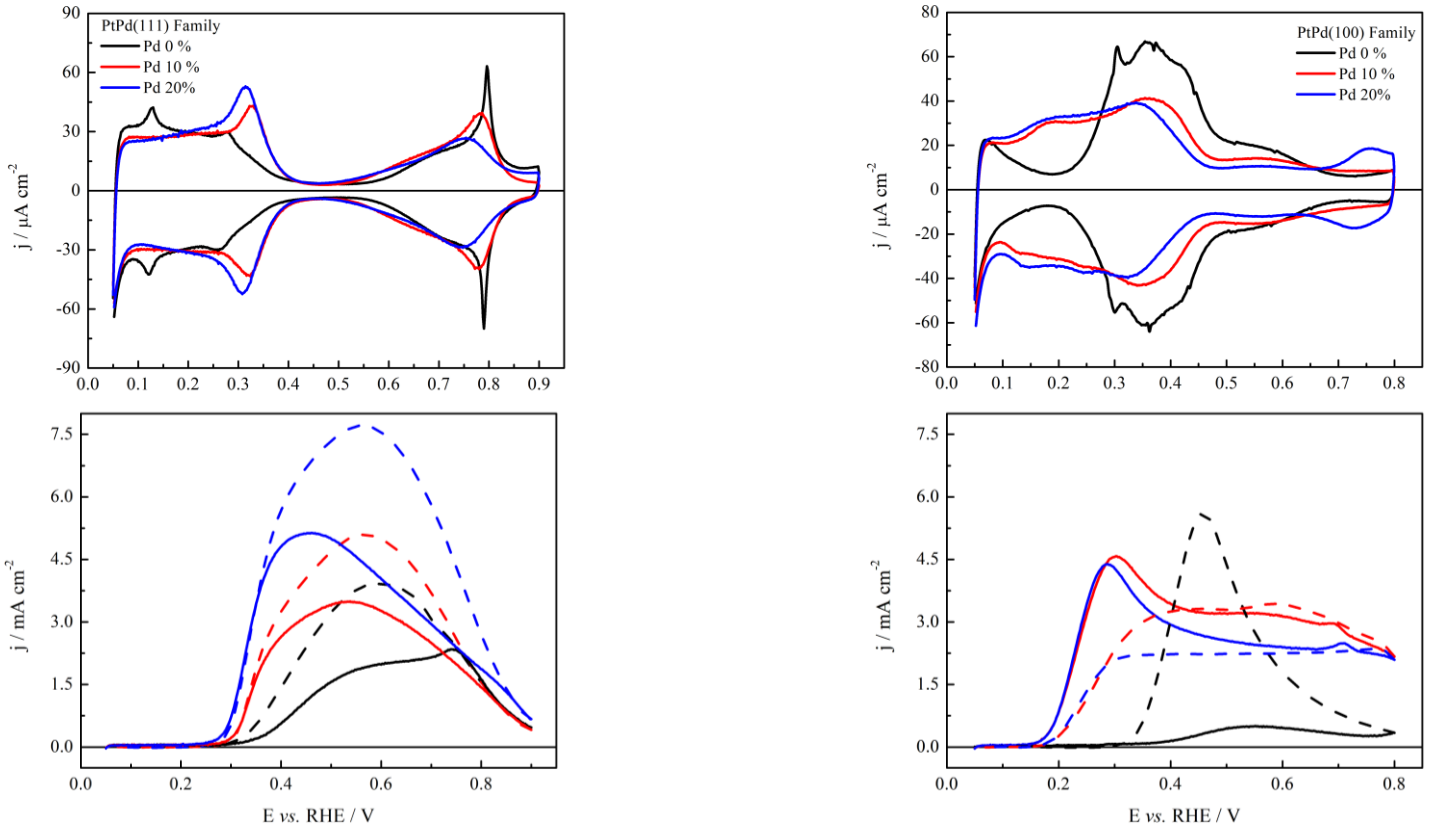


Fig. 4 – FAEOR on Pt(111) or PtPd(111) Family in acid or alcaline medio. Solid and dotted lines represent positive and negative going scans, respectively. $|dE/dt| = 0.05\ V\ s^{-1}$; $[HClO_4]$ and $[NaOH] = 0.1\ mol\ L^{-1}$.

Acknowledgment

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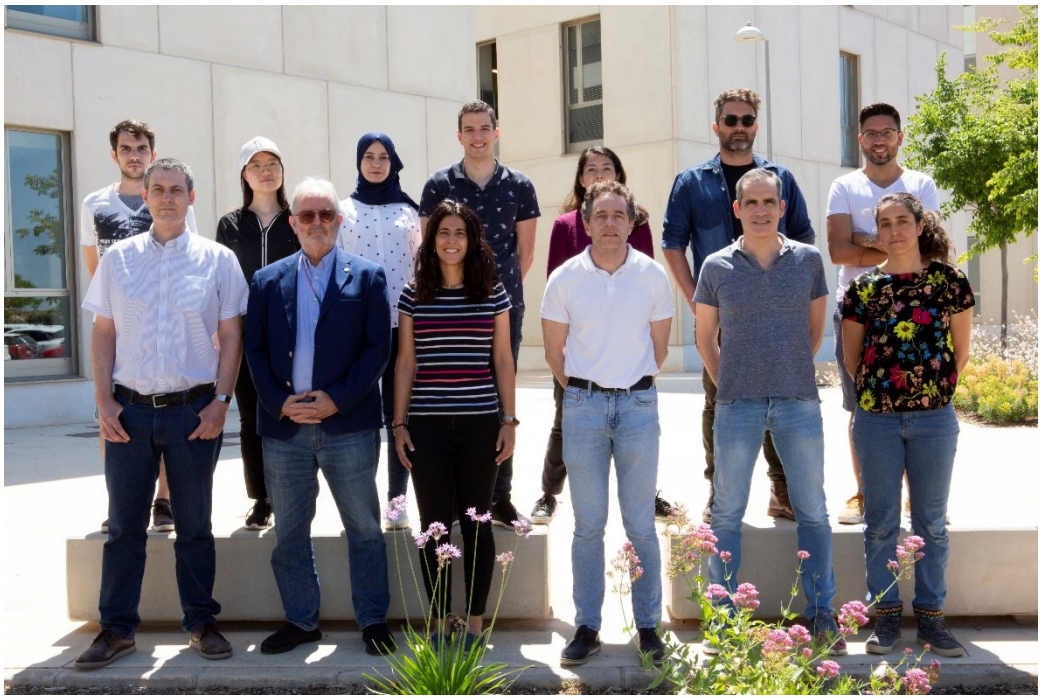
SURFACE ELECTROCHEMISTRY GROUP



Thank You !!!

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Director: Rosa M. Arán-Ais

Santander, 6 - 8 de Julio de 2022