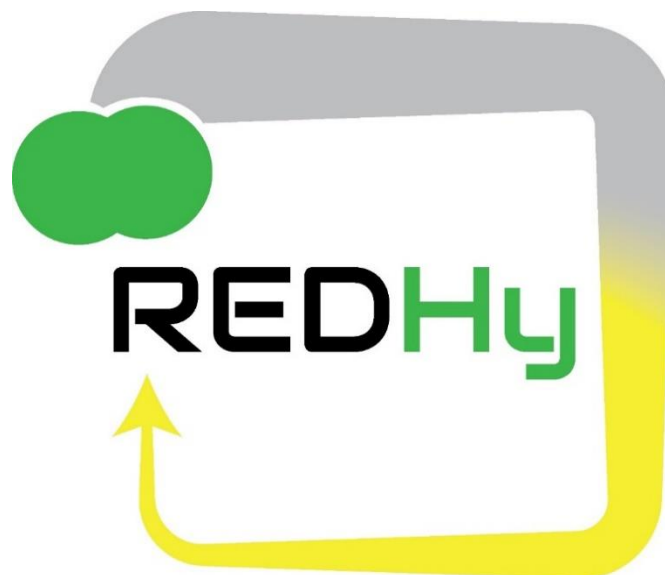


**HORIZON EUROPE PROGRAMME**  
**TOPIC HORIZON-CLEANH2-2023-01-01**

**GA No. 101137893**


# **REDHY**

**Redox-Mediated economic, critical raw material free,  
low capex and highly efficient green hydrogen  
production technology**



## **REDHY - Deliverable report**

### **D2.1 – Theoretical Calculations**

<b>Deliverable No.</b>	2.1	
<b>Related WP</b>	WP2	
<b>Deliverable Title</b>	Theoretical Calculations	
<b>Deliverable Date</b>	27/08/2025	
<b>Author(s)</b>	Germán Sastre, Sara Goberna (UPV)	
<b>Checked by</b>	Steering Committee	
<b>Reviewed by (if applicable)</b>	All Partners	
<b>Approved by</b>	Tobias Morawietz (DLR)	
<b>Status</b>	Final	

## Document History

Version	Date	Editing done by	Remarks
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## Public Summary

In WP2, the synthesis, intentional modification, and assessment of the redox performance of two types of redox mediators will be conducted using suitable carbon electrodes to enhance the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). Task 2.1 involves theoretical calculations to determine the redox potentials of proposed molecules and complexes. Deliverable 2.1. involves reporting of summarized DFT calculations.

### 3 Acknowledgement

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#### Project partners:

#	Partner short name	Partner Full Name
1	DLR	DEUTSCHES ZENTRUM FÜR LUFT – UND RAUMFAHRT EV
2	CNRS	<u>CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE</u>
3	UNR	<u>UNIRESEARCH BV</u>
4	UPV	<u>UNIVERSITAT POLITECNICA DE VALANCIA</u>
5	IDN	<u>INDUSTRIE DE NORA SPA-IDN</u>
6	CENMAT	<u>CUTTING-EDGE NANOMATERIALS CENMAT UG HAFTUNGSBESCHRÄNKT</u>
7	CNR	<u>CONSIGLIO NAZIONALE DELLE RICERCHE</u>

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