Ministero dell'Università e della Ricerca

Segretariato Generale
Direzione generale della ricerca

IL DIRETTORE GENERALE

VISTO il Decreto-legge del 9 maggio 2020 n. 1 pubblicato nella Gazzetta Ufficiale n. 6 del 9 gennaio 2020 istitutivo del Ministero dell'Università e della Ricerca (MUR), convertito con modificazioni in Legge 5 marzo 2020, n. 12, pubblicato nella Gazzetta Ufficiale n. 61 del 9 marzo 2020 ed in particolare l'art.4 comma 1 dello stesso;

VISTO il Decreto del Presidente del Consiglio dei Ministri 30 settembre 2020, n. 164 rubricato "*Regolamento concernente l'organizzazione del Ministero dell'Università e della Ricerca*" pubblicato in GU Serie Generale n. 309 del 14.12.2020; in particolare l'art.11 comma 1, del predetto decreto di organizzazione il quale prevede "*Il Ministero provvede al conferimento degli incarichi per le posizioni dirigenziali generali e non generali oggetto di riorganizzazione ai sensi del presente decreto, seguendo le modalità, le procedure e i criteri previsti dall'articolo 19 del decreto legislativo 30 marzo 2001, n. 165*";

VISTO il Decreto del Ministro dell'Università e della Ricerca del 19 febbraio 2021, pubblicato nella Gazzetta Ufficiale del 26 marzo 2021 n.74, recante "*Individuazione e definizione dei compiti degli uffici di livello dirigenziale non generale del Ministero dell'Università e della Ricerca*";

VISTA la Legge 7 agosto 1990, n. 241 "*Nuove norme in materia di procedimento amministrativo e di diritto di accesso ai documenti amministrativi*" e ss.mm.ii.;

VISTO l'articolo 1, comma 312, della Legge 30 dicembre 2021, n. 234 "Bilancio di previsione dello Stato per l'anno finanziario 2022 e bilancio pluriennale per il triennio 2022-2024", che istituisce il "Fondo italiano per le scienze applicate" (di seguito FISA);

VISTO l'articolo 11 della legge 16 gennaio 2003, n. 3, come modificato dall'articolo 41 del Decreto-legge del 16 luglio 2020, n. 76, convertito con modificazioni dalla legge 11 settembre 2020, n. 120, che prevede la nullità degli atti amministrativi, anche di natura non regolamentare, che dispongono il finanziamento pubblico o autorizzano l'esecuzione di progetti di investimento pubblico in assenza dei corrispondenti CUP che costituiscono elemento essenziale dell'atto stesso;

VISTA la delibera del CIPE n. 63 del 26 novembre 2020 che introduce la normativa attuativa della riforma del CUP;

VISTA l'Anagrafe nazionale delle ricerche (ANR), istituita e disciplinata con Decreto del Presidente della Repubblica n. 382 dell'11 luglio 1980, nonché con i decreti del Ministro dell'università e della ricerca, nn. 564/2021 e nn. 615/2021;

VISTO il Regolamento (UE) 2018/1046 del 18 luglio 2018, che stabilisce le regole finanziarie applicabili al bilancio generale dell'Unione, che modifica i Regolamenti (UE) n. 1296/2013, n. 1301/2013, n. 1303/2013, n. 1304/2013, n. 1309/2013, n. 1316/2013, n. 223/2014, n. 283/2014 e la decisione n. 541/2014/UE e abroga il regolamento (UE, Euratom) n. 966/2012;'

VISTA la Comunicazione della Commissione 2014/C 198/01 "*Disciplina degli aiuti di Stato a favore di ricerca, sviluppo e innovazione*" e ss.mm.ii.;

VISTO il Regolamento (UE) General Block Exemption Regulation (GBER) n. 651/2014 della Commissione, del 17 giugno 2014 e ss.mm.ii., che dichiara alcune categorie di aiuti compatibili con il mercato interno in applicazione degli articoli 107 e 108 del trattato;

VISTA la Comunicazione della Commissione del 19 marzo 2020, C(2020) 1863 "*Quadro temporaneo per le misure di aiuto di Stato a sostegno dell'economia nell'attuale emergenza della COVID-19*", da ultimo rettificata attraverso la comunicazione del 18 novembre 2021, C(2021) 8442 final "*Sesta modifica del quadro temporaneo per le misure di aiuto di Stato a sostegno dell'economia nell'attuale emergenza della COVID-19 e modifica dell'allegato della comunicazione della Commissione agli Stati membri sull'applicazione degli articoli 107 e 108 del trattato sul funzionamento dell'Unione europea all'assicurazione del credito all'esportazione a breve termine*";

VISTA la comunicazione della Commissione 2016/C 262/01 sulla nozione di aiuto di Stato di cui all'articolo 107, paragrafo 1, del trattato sul funzionamento dell'Unione europea;

VISTO il Decreto del Ministro dell'Università e della Ricerca del 14 dicembre 2021, n. 1314, recante "Disposizioni per la concessione delle agevolazioni finanziarie", successivamente modificato con Decreto Ministeriale 24 dicembre 2021, n. 1368;

VISTO il Decreto del Ministro dell'Università e della Ricerca, di concerto con il Ministro dello Sviluppo Economico, n. 327 del 29 marzo 2022, registrato alla Corte dei Conti in data 26 aprile 2022 n. 1139, con il quale, in attuazione delle disposizioni del richiamato articolo 1, comma 312, della Legge 30 dicembre 2021, n. 234, sono stati stabili criteri e modalità di assegnazione delle risorse del FISA;

VISTO il Decreto del Ministro dell'Università e della Ricerca, di concerto con il Ministro dello Sviluppo Economico, n. 582 del 24 giugno 2022, registrato alla Corte dei Conti in data 20 luglio 2022 n. 1924, con il quale, in attuazione delle disposizioni dell'articolo 9 del predetto Decreto n. 327 del 29 marzo 2022, è stata istituita la ivi prevista Cabina di Regia per le attività di indirizzo delle iniziative, di approvazione degli Avvisi e le successive attività di monitoraggio dei risultati e delle ricadute delle proposte finanziate;

VISTO il Decreto MEF del 31 dicembre 2021 di Ripartizione in capitoli delle Unità di voto parlamentare relative al bilancio di previsione dello Stato per l'anno finanziario 2022 e per il triennio 2022-2024 che, nell'ambito della missione n. 17 "Ricerca e innovazione", al programma n. 22 "Ricerca scientifica e tecnologica di base e applicata" prevede al capitolo 7725 piano gestionale 01 lo stanziamento per l'anno 2022 del "Fondo Italiano per le Scienze Applicate (FISA)";

VISTE le disponibilità in termini di competenza sul capitolo 7725 per l'esercizio 2022, pari a € 50.000.000,00, di cui il 2 per cento destinato all'attività di valutazione;

VISTO il Decreto Direttoriale del 13 settembre 2022, n. 1405 di emanazione di un *"Avviso per la presentazione di proposte progettuali"* (di seguito *Avviso*) con le risorse del predetto FISA per l'anno 2022;

CONSIDERATO che le aree previste dall'avviso sono: *1. Agriculture - Rural Development – Fisheries, 2. Biotechnology; 3. Construction, Civil engineering, Infrastructures; 4. Consumer products and services; 5. Earth and related environmental sciences; 6. Education and Culture; 7. Energy; 8. Engineering and technology; 9. Food and beverages; 10. Health; 11. Information and Communication Technology (ICT); 12. Public sector innovation; 13. Security; 14. Space; 15. Transport & Mobility***;**

VISTE le domande presentare nel rispetto dei tempi e nelle modalità previste nell'Avviso, per un totale di n. 482 proposte progettuali di cui n. 22 riferibili all'area "*Energy*";

TENUTO CONTO degli esiti della valutazione tecnico-scientifica e di quella sulla capacità economico-finanziaria, di cui all'art. 7 dell'Avviso;

VISTO il Decreto Direttoriale n. 842/2023 , con il quale è stata approvata la graduatoria delle proposte pervenute per l'area "*Energy*", con contestuale ammissione alla successiva Fase di negoziazione delle proposte risultate idonee, ai sensi degli artt. 3, 4, 5 dell'Avviso;

VISTO il Decreto Ministeriale 1457 del 20 ottobre 2023, con il quale è stata nominata, in coerenza con quanto stabilito dall'articolo 8, comma 2, dell'Avviso, la Commissione per la Fase Negoziale;

VISTO l'esito della fase negoziale condotta dalla Commissione di cui al punto precedente in base a quanto disposto dall'articolo 8 dell'Avviso;

VISTO il Decreto Direttoriale n. 152/2024 con il quale sono state individuate le proposte finanziabili per l'area "*Energy*" , registrato alla Corte Dei Conti in data 02 Aprile 2024 con il n. 714;

VERIFICATA la corretta finalizzazione della documentazione esecutiva dell'intervento in coerenza con quanto previsto dall'articolo 8, comma 4, dell'Avviso;

DATO ATTO che gli obblighi di cui all'art. 11, comma 3, del Decreto Ministeriale n. 1314 del 2021 e ss.mm.ii., sono stati assolti mediante l'avvenuta iscrizione del Progetto approvato, e dei soggetti fruitori delle agevolazioni, nell'Anagrafe nazionale della ricerca;

VISTO il Decreto Legislativo del 6 settembre 2011 n. 159 "Codice delle leggi antimafia e delle misure di prevenzione, nonché nuove disposizioni in materia di documentazione antimafia, a norma delgli articoli 1 e 2 della legga 13 agosto 2010, n. 316" e ss.mm.ii. e atteso che il perfezionamento della contrattualizzazione è subordinato all'espletamento di tutti gli adempimenti allo stesso collegati;

VISTI i Codici di Progetto (CUP), di cui all'art. 11 della Legge gennaio 2003, n. 3;

VISTO l'appunto a firma del Responsabile Unico del Procedimento con il quale viene sottoposto alla firma il presente decreto;

RITENUTO che nulla osti all'adozione del provvedimento di concessione del finanziamento del Progetto FISA-2022-00277;

DECRETA

Articolo 1

1. È ammessa al finanziamento, nell' ambito di intervento "*Energy*", la domanda di agevolazione contrassegnata dal codice identificativo FISA-2022-00277, per la realizzazione del Progetto dal titolo "*SCOOP-Novel Solar cells for solar-to-hydrogen COntinuOus Production*".

2. I termini, le condizioni, le forme, le misure, le modalità di attuazione e gli obblighi di rendicontazione del Progetto finanziato sono indicati nella normativa citata in premessa e nei seguenti documenti: **Allegato A** – Capitolato Tecnico; **Allegato B** – Piano dei Costi; **Allegato C**– Cronoprogramma di attuazione; **Allegato D** – Disciplinare di concessione delle agevolazioni.

3. I Codici Unici di Progetto (CUP) rilasciati dal Registro Nazionale degli Aiuti di Stato ai sensi del citato D.M. 31 maggio 2017, n. 115 e ss.mm.ii (inserire solo se necessario), riferiti ad ogni singolo Soggetto beneficiario, sono riportati nell'**Allegato E** - Codici Unici di Progetto (CUP) che costituisce parte integrante del presente Decreto.

Articolo 2

1. Le risorse necessarie per gli interventi del Progetto di cui all'art. 1 del presente Decreto Direttoriale, sono determinate complessivamente in € 1.896.578,66 (unmilioneottocentonovantaseimilacinquecentosettantotto/66), nella forma del contributo diretto alla spesa, nei limiti delle intensità massime di aiuto stabilite dall'articolo 25 del Regolamento GBER.

2. La somma indicata al precedente comma 1 verrà erogata dal MUR, nel rispetto della normativa vigente e delle disposizioni previste dal D.M. 14 dicembre 2021, n. 1314 e ss.mm.ii., e in base al Cronoprogramma di attuazione e Piano dei pagamenti di cui agli Allegati B e C.

3. L'avvio delle attività di rendicontazione resta subordinata alla conclusione delle procedure di accettazione del Disciplinare (Allegato D) e sottoscrizione dell'Atto d'Obbligo conseguenti l'adozione del presente Decreto Direttoriale di concessione.

Il presente Decreto è trasmesso agli Organi di controllo per i seguiti di competenza e sarà pubblicato nelle rituali forme di legge.

Allegati

- Allegato A – Capitolato Tecnico;
- Allegato B – Piano dei Costi;
- Allegato C- Cronoprogramma di Attuazione;
- Allegato D - Disciplinare di concessione delle agevolazioni;
  - Allegato E - Codici Unici di Progetto (CUP).

IL DIRETTORE GENERALE
(Dott. Vincenzo Di FELICE)

Firmato digitalmente da DI FELICE VINCENZO
C=IT
O=MINISTERO DELL'UNIVERSITA' E DELLA RICERCA

FONDO ITALIANO PER LE SCIENZE APPLICATE (FISA)

ALL. A

CAPITOLATO TECNICO DEFINITIVO

Novel Solar cells for solar-to-hydrogen COntinuOus Production (SCOOP)

Università degli Studi di Messina, Italy

prof.s Siglinda PERATHONER

FISA-2022-00277, Macro Area ENERGY

Updated to reflect the changes in the budget during negotiation

OUTLINE

Synopsis

SCOOP addresses the main challenges of **i**) discontinuity in using sunlight as a renewable energy source[1] and **ii**) producing green H_2 at lower costs than electrolysis.[2, 3] Sun represents the energy future for Sicily,[4] but this scenario cannot be realised without converting it to fuels (e.g. solar fuels) for energy storage and distribution. Green H_2 is another major challenge for Sicily (and Italy) to decarbonise production,[5] but when the current high electrolysis costs are overcome. This could be realised by developing solar panels producing hydrogen directly from sunlight and water. Still, it requires realising a continuous (24h) production of H_2 to avoid costs for H_2 storage.

SCOOP addresses both these challenges with a revolutionary approach in which an electrocatalytic (EC) cell is coupled to a photovoltaic (PV) module, with the PV-driven EC cell able to convert CO_2 and water to a mixture of H_2 and formic acid (FA). The latter is an intermediate storage chemical used to generate H_2 during dark periods, forming back CO_2, which can be recirculated. The concept is schematically presented in Figure 1.

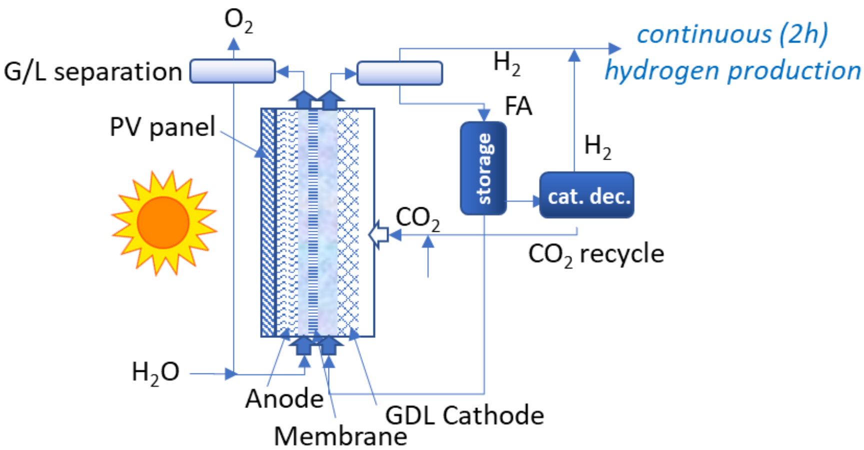


Figure 1 Schematic illustration of the solar cell for continuous (24h) production of hydrogen proposed by the SCOOP project.

The cell results from an EU project (A-LEAF, ID#732840, ended 6/2021), where the UniME group developed and engineered the cell up to TRL 3, obtaining world-record results in terms of combined solar-to-fuel (STF) efficiency and current density using only earth-abundant materials for cell materials. Figure 2 presents a view of the TRL 3 cell realised in the frame of this A-LEAF project and of the results obtained compared to state-of-the-art literature results.

Still, the A-LEAF project focused on converting CO_2 to FA rather than using FA as an intermediate storage element to realise continuous H_2 production. Thus, the SCOOP project starts from the A-LEAF TRL 3 results but gives a new applicative perspective.

SCOOP will do

- Non-predominant *fundamental* research to optimise electrodes and cell design to enhance further STF, stability and productivity,
- *Prevailing industrial* research for **2.a**) scaling up to TRL 5-6 the cell, **2.b**) testing its stability, **2.c**) integrating the unit to decompose FA catalytically during dark periods to have a continuous (24h) production of H_2, **2.d**) evaluate the techno-economic costs of H_2 production, and assess the impact by LCA.
- Non-predominant *experimental* development centred on creating a *Solar Fuel Hub*. It will act as the showcase to disseminate the project results to stakeholders and the public and to increase visibility on the use of solar energy and green H_2.

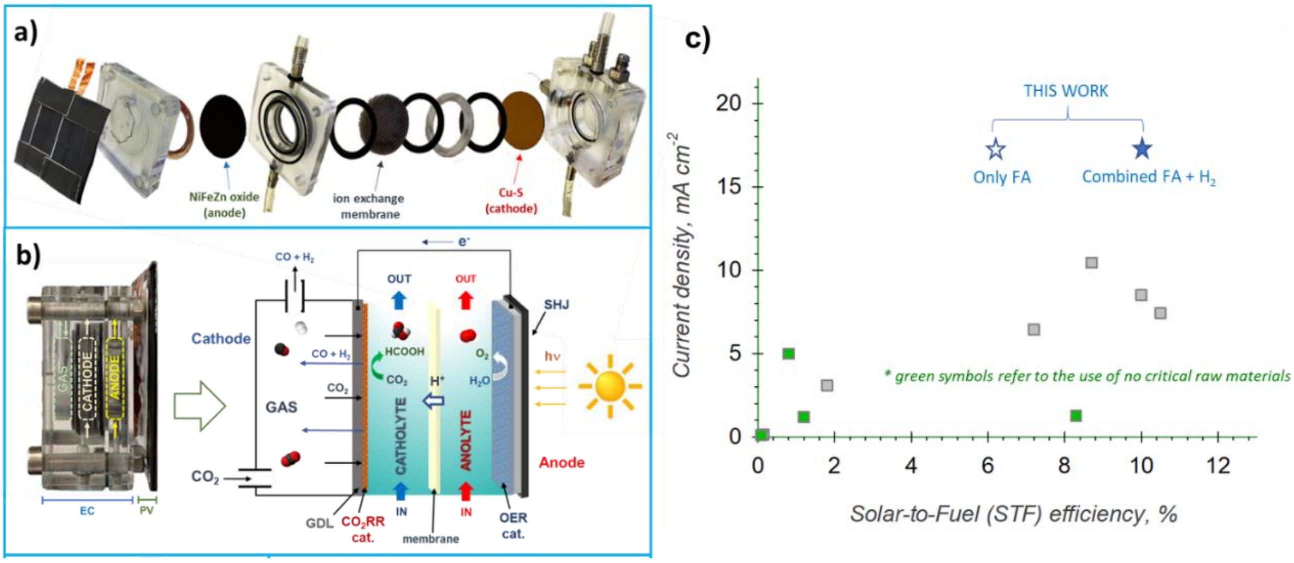


Figure 2 From the previous EU project (A-LEAF) on which the SCOOP project starts as TRL 3. **a**): Exploded view of the electrochemical (EC) – photovoltaic (PV) device and related electrodes (based only on earth-abundant materials); **b**) scheme of working principle of the cell (leading to the combined production of FA and H_2 from water, CO_2 and sunlight, without external bias or sacrificial agents) with a picture of the fully-integrated cell; **c**) presentation of the world-record performances in terms of combined current density and solar to fuel efficiency obtained by this cell in comparison with state-of-the-art literature results.

Motivations, Relevance and Long-term Vision

Sicily is a region of Europe with the largest potential for renewable energy production.[1] Still, it can be exploited only for a reduced fraction because transporting renewable energy to the Nord of Italy is inefficient. In addition, the discontinuity of production creates major issues in balancing the demand. Current storage systems for electrical energy, including batteries, are still inefficient.[6]

Using suitable vectors such as hydrogen in energy-intensive industries[7] is commonly identified as necessary to realise significant decarbonisation and substitution of fossil fuels. Green H_2 should be used, but producing it by electrolysis is still largely the only available solution.[8] However, this energy-intensive process requires over 70% renewable electrical energy to decrease the carbon footprint effectively.[9, 10] This is available currently in the grid (and similarly for at least the next one-two decade) for only a short fraction of the day, with thus a large increase in Capex (capital expenditure) of electrolysers.

The alternative is to realise dedicated solar fields in regions with high solar irradiation, such as Sicily, where the solar photovoltaic (PV) panels are integrated with an electrocatalytic (EC) unit where the H_2 is coproduced with a storage element, such as formic acid, which can be decomposed during dark periods to form H_2. This novel approach will chemically store H_2 as FA during the light period and then decompose FA during the dark period for a continuous (24h) production of H_2.

This solution may lead to the development of an artificial leaf (AL) type device, which then can be integrated with others to form an artificial tree for thus a distributed production of H_2. Figure 3 presents a pictorial view of the AL-type devices and assembling to form an artificial tree that uses sunlight and water to produce H_2 in a distributed, virtually zero-impact manner. *This longer-term vision is beyond the scope of the SCOOP project*, which is to demonstrate the feasibility of the concept at TRL5-6. However, it illustrates the long-term perspective and the high social and visual impact of changing the modality to produce hydrogen as a clean energy vector.

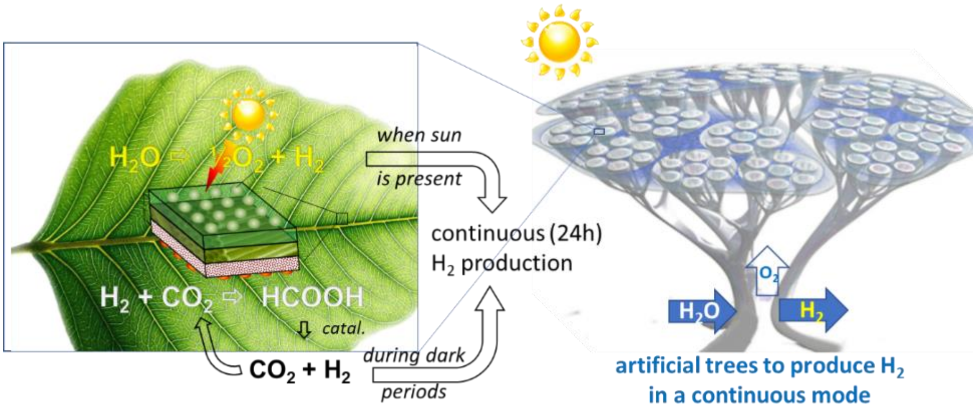


Figure 3 Pictorial representation of the AL-type device developed within the SCOOP project and how it can be integrated with other units to form an artificial tree to produce H_2 continuously using sunlight and water. It pictorially illustrates the high social impact the project may have in changing the modality to produce hydrogen as a clean energy vector.

Key qualification elements of the proposal

EVALUATION CRITERIA*	SCOOP characterising aspects
a) quality (including the scientific quality and that relating to the experiences of exploiting the results) of the PIs, the Beneficiaries, and all other subjects possibly involved in the project activities	- experience and competences of (i) the PI: pag.s 6-8, (ii) the host Institutions and groups involved: see pag.s 9-11, (iii) beneficiary(ies) and other Institutions involved in the project, pag.s 11-12
b) autonomy and decision-making, organisational and coordination capacity of the PI concerning all the subjects participating in the project proposal	- autonomy and decision-making, organisational and coordination capacity of the PI: pag.s 6-8, 12-13
c) innovativeness and originality of the proposal to the international state of the art	- innovativeness and originality of the proposal: pag.s 3-5, 14, 26-29 - project description and organization: pag.s 15-23
d) relevance of the proposal in terms of repercussions and socio-economic impact	- relevance and impact: see pag.s 4-5, 23, 25, 29-37
e) ability of the proposal to introduce significant and competitive product and/or process and/or service innovations in the indicated time frame and in the social, economic, industrial context of reference	- competitiveness to the social, economic, and industrial context of reference: pag.s 25, 29-37
f) congruity of the economic characteristics of the proposal and share of co-financing to be paid by private subjects	- congruity of the economic requests: - share of co-financing to be paid by private subjects: this is a single PI and partner project, according to the call, and thus without co-financing
***** *from the announcement*	

According to the call indications, the SCOOP proposal is presented by **one** individual researcher (Principal investigator) together with a *single* Hosting Institution. The project has predominant Industrial Research and non-predominant Fundamental Research and Experimental Development activities.

SECTION 1

Experience and competencies of the Principal Investigator (PI)

The *Principal Investigator* is prof.sa **Siglinda PERATHONER**, who is a full professor of Industrial Chemistry at the University of Messina (Italy) and Director of the centre **CASPE** (*Laboratory of Catalysis and Sustainable Production and Energy*), a joint centre between the University of Messina, the Interuniversity Consortium INSTM (Science & Technology of Materials, a main research consortium in Italy) and ERIC aisbl (European Research Institute of Catalysis, Brussels, Belgium). The research in this proposal will be mainly done at this centre.

Research Profile of PI

She was starting from the initial background on the photophysics of supramolecular complexes with prof. V. Balzani and the Nobel Laureate J.M. Lehn. Then, the scientific focus of prof. Perathoner moved to the industrial development of catalytic materials and processes initially for environmental applications (water emissions, NOx abatement in stationary and mobile emissions) and then for sustainable energy and chemical production, particularly electro- and photo-catalytic applications, H_2 production from waste, energy materials based on nanocarbon.

Her research interests include nanostructured oxides, micro-/meso-porous materials and nanocarbons for catalytic applications, using solar energy to convert small molecules (CO_2, H_2O and N_2). While dedicating attention to fundamental aspects and the reaction mechanisms, the core of the activities was on transferring **basic research into practical applications**. The most significant part of the research was made in the frame of **European projects involving many companies**, in various cases also coordinating the projects. Four prototype or pilot industrial units for electrocatalytic processes were realised. Various waste-to-H_2 plants are in construction.

Among the **pioneering activities**, the development of **1**) electrocatalysts for the direct electroreduction of CO_2 to C2-C3 hydrocarbons/alcohols (among the reporting this possibility already over 15 years ago), **2**) artificial-leaf type devices for CO_2 reduction (with now world-record solar-to-fuel efficiencies of over 10% at high current density), **3**) electrolyte-less electrocatalytic devices (now becoming of broad use to overcome limitations of the current devices), **4**) electrodes based on ordered arrays of TiO_2 nanotubes for photo- and electrocatalytic reactions, **5**) metal-free nanocarbons for catalytic and electrocatalytic applications, **6**) catalytic solutions for carbon circularity (CO_2 reuse), **7**) a process to produce H_2 from municipal waste (implemented on an industrial scale) and the use of **8**) iron-oxide on nanocarbons electrocatalysis for the N_2 electrocatalytic conversion to ammonia.

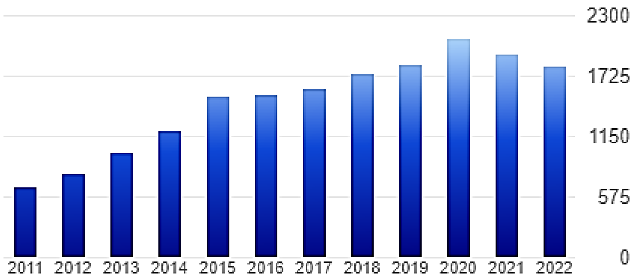
In parallel with the scientific developments, intense activity was also made in perspective papers, leading to highly cited pioneering manuscripts on nanocarbons, layered materials, CO_2 recycling and utilisation, solar fuels and artificial leaf, and fossil-free chemical production. In addition, she is editor of three **books** on Sustainable Industrial Chemistry, Green Carbon Dioxide and contributions to encyclopaedias.

- **CURRENT POSITION(S)**

2018 – today Full Professor (Industrial Chemistry), Univ. Messina - Italy, Dept. ChiBioFarAm
2018 – today Coordinator of the Laboratory of Catalysis and Sustainable Production and Energy (CASPE), reference centre of the Interuniversity Consortium INSTM (Science & Techn. of Materials).

- **Research Output (summary of publication record)**

- Over **430** papers in peer-reviewed journals (IRIS official database of the Univ. Messina: 325 publications, 96 book chapters and 14 monographs), *>220 in last 10 years*.
- **H-index: 76** (50 from 2017), *>24000 citations* (~11000 from 2017), *54 papers cited ≥100 times*, 282 papers cited ≥10 times (Google Scholar, Sept. 2022); h-index (last 10 years) = 42 (IRIS Cineca Database), 40 (Scopus)
- *Qualification of peer-reviewed articles (IRIS)*: *WoS Average*



IF5Y= 6,327 *Max*. IF5Y=48,832, WoS Average Citations= 47,169 Max. Citations= 905
- *SciVal (Elsevier - Scopus, 2011-2020)*: 43.2 average nr citations per public., 21 patents citing, 123.5 average Patent-Citations per 1,000 Scholarly Outputs, 37.1% Intern. collaboration, Top collaborating Institutions: Chinese Academy of Sciences (13 public.), CNRS (12 publ.), Max Planck Society (11 publ.), Inst. of Metal Research – China (10 publ.).
- 11 plenaries, 5 keynotes, > 20 invited in the last 10 years
- Chairperson in international conferences: 6 in years 2011-2021
- Editor of books and special issues of international journals: 6 in years 2011-2021
- Monographs and Encyclopedia: 3 in years 2011-2021 + 1 international roadmap on catalysis
- *Recognised industrial innovation leadership*: award from S.C.I., Levi Medal
- Full list of publications: link

- **Qualification**

- *Top Italian Scientists*: among the top 5 female researchers in chemistry working in Italy (as h-index)
- *SciVal (Elsevier – Scopus, 2011-2020):* 245% and 140% increase to the world average for chemistry in Field-Weighted Views and Citation, respectively
- *SciVal (Elsevier - Scopus, 2011-2020)*: 153 publ., 73,2% in Q1 (CiteScope), 47.1% in top 10% and 10% in top 1% journals, 19,356 Scopus views (64.1% in top 10% most viewed)

- **Ten Representative Publications**

i) G Papanikolaou, G Centi, S Perathoner, P Lanzafame, Catalysis for e-Chemistry: Need and Gaps for a Future De-Fossilized Chemical Production, with Focus on the Role of Complex (Direct) Syntheses by Electrocatalysis, *ACS Catalysis* **2022**, 12 (5), 2861-2876. *IF: 13.7, Citations (Sept 22): 7*

ii) G Centi, S Perathoner, Redesign chemical processes to substitute the use of fossil fuels: A viewpoint of the implications on catalysis, *Catal. Today*. **2022**, 68, 216-223. *IF: 6.6, Citat. (Sept 22): 7* 🏆 *Top 1% cited*

iii) R Arrigo, R Blume, V Streibel, C Genovese, A Roldan, ME Schuster, C Ampelli, S Perathoner, JJ Velasco Vélez, M Hävecker, A Knop-Gericke, R Schlögl, G Centi, Dynamics at Polarized Carbon Dioxide–Iron Oxyhydroxide Interfaces Unveil the Origin of Multicarbon Product Formation, *ACS Catal*. **2021**, 12 (1), 411-430. *IF: 13.7, Citations (Sept 22): 6*

iv) G Centi, S Perathoner, Nanocarbon for Energy Material Applications: N_2 Reduction Reaction, *Small* **2021**, 17 (48), 2007055. *IF: 15.2, Citations (Sept 22): 13*

v) D Giusi, C Ampelli, C Genovese, S Perathoner, G Centi, A novel gas flow-through photo-catalytic reactor based on copper-functionalised nanomembranes for the photoreduction of CO_2 to C1-C2 carboxylic acids and C1-C3 alcohols, *Chem. Eng. J*. **2021**, 408, 127250. *IF: 16.7, Citations (Sept 22): 22*

vi) V Romano, G D'Angelo, S Perathoner, G Centi, Current density in solar fuel technologies, *Energy & Env. Sci*. **2021**, 14 (11), 5760-5787. *IF: 39.7, Citations (Sept 22): 12*

vii) H Wei, Q Jiang, C Ampelli, S Chen, S Perathoner, Y Liu, G Centi, Enhancing N_2 Fixation Activity by Converting Ti_3C_2 MXenes Nanosheets to Nanoribbons, *ChemSusChem* **2020**, 13 (21), 5614-5619. *IF: 9.3, Citations (Sept. 22): 16 (Cover)*

viii) S Chen, S Perathoner, C Ampelli, H Wei, S Abate, B Zhang, G Centi, Enhanced performance in the direct electrocatalytic synthesis of ammonia from N_2 and H_2O by an in-situ electrochemical activation of CNT-supported iron oxide nanoparticles, *J Energy Chem*. **2020**, 49, 22-32. *IF: 13.6, Citations (Sept 22): 29*

ix) C Genovese, ME Schuster, EK Gibson, D Gianolio, V Posligua, R Grau-Crespo, G Cibin, PP Wells, D Garai, V Solokha, S K Calderon, JJ Velasco-Velez, C Ampelli, S Perathoner, G Held, G Centi, R Arrigo, Operando spectroscopy study of the carbon dioxide electro-reduction by iron species on nitrogen-doped carbon, *Nature Comm*. **2018**, 9 (1), 1-12. *IF: 17.7, Citations (Sept 22): 148*

x) Y Lin, X Sun, DS Su, G Centi, S Perathoner, Catalysis by hybrid sp^2/sp^3 nanodiamonds and their role in the design of advanced nanocarbon materials, *Chem. Soc. Rev*. **2018**, 47 (22), 8438-8473. *IF: 60.6, Citations (Sept 22): 102*

- **Lectures (plenary, keynote, invited) at intern. conferences and companies (selection, last 5Y)**

- Bridging nanoscience and electrocatalysis to design advanced electrodes, 44th Int Conference on Coord. Chem., Au. 28th- Sept. 2th, 2022, Rimini, Italy. *Invited*
- Electrocatalysis: facing the challenge of extending its use to go beyond fossil fuels, Europacat 2021, Prague, Czech Rep., 29/08-3/09 2021, *keynote* (postponed 2023)
- The New C2 Value Chain from CO_2 Electrocatalytic Reduction, E.U. Green Week, Bruxelles, Belgium. 04/06 2021, *invited*.

- Production of Solar Fuels Using CO_2, SINCHEM Winter School 2020, 4-6, 2020 Bologna, Italy; *plenary*.
- Photoelectrocatalytic (PEC) solar cells not containing critical raw materials to reduce CO_2. First International Bunsen-Discussion-Meeting on Fundamentals and Applications of (Photo) Electrolysis for Efficient Energy Storage, April 1 – 5, 2019, in Taormina, Italy; *invited*.
- Oxidative dehydrogenation over nanocarbons: recent mechanistic study, CARBOCAT VIII - 8th Int. Symp. on Carbon for Catalysis, Porto (Portugal), 26th-29th June 2018, *keynote*
- Photo- and Electrocatalytic Approaches for a Renewable Energy-Driven Chemistry and Energy, Ernst Haage Symposium, November 22-24, 2017, Mülheim - Germany, *plenary*
- Catalysis for the changing scenario for sustainable energy and chemistry production CIS-7 (7th Czech Italian-Spanish Symposium on Catalysis), June 13-17th 2017, Trest (Czech Rep.), *plenary*

- **Monographs and Encyclopaedia (last 10 years)**

2021 G. Centi, S. Perathoner, **Handbook of Climate Change Mitigation and Adaptation**. Springer. (Entry 1: Catalytic Technologies for the Conversion and Reuse of CO_2, 50 pages; DOI: 10.1007/978-1-4614-6431-0_119-1; Entry 2: Reduction of non-CO_2 Greenhouse Gas Emissions by Catalytic Processes, 44 pages, DOI: 10.1007/978-1-4614-6431-0_49-3)

2016 S. Perathoner, G. Centi, **Science and Technology Roadmap on Catalysis for Europe**, *European Cluster on Catalysis*, ERIC Pub., Brussels 2016, ISBN 979-12-200-1453-3

2014 G. Centi, S. Perathoner, *Artificial Leaves*, **Kirk-Othmer Encyclopedia of Chemical Technology**, Wiley, April 2014, DOI: 10.1002/0471238961.articent.a01

2013 G. Centi, S. Perathoner, *Mixed-metal oxides*, **Comprehensive Inorganic Chemistry II** (Vol. 7), 31 pages, Elsevier 2013, DOI:10.1016/B978-0-08-097774-4.00718-X

- **FELLOWSHIPS, AWARDS AND RECOGNITIONS**

2021 CAS (Chinese Academy of Sciences) President's International Fellowship Initiative, PIFI. (Visiting Scientists)

2021 Mario Giacomo Levi Medal of the Italian Chemical Society for the innovative activity carried out in the field of Chemistry that led to industrial implementation

2021-22 World's top 2% scientists, according to the Stanford University ranking

2021 Member of the ASN (Italy) and ERC (EU) evaluation panels

2011 "NanoInLife", a film produced by the European Commission to show the public the results of nanotechnologies; interview with S. Perathoner and presentation of the results on CO_2

2010 Finalist of the European Sustainable Chemistry Award 2010 (EuCheMS)

2008 "Altran Foundation for Innovation", a special award for the project on the development of artificial trees for the conversion of CO_2

2006 EU ELCAT project (coord. S. Perathoner): selected among EU success stories, one of the eight projects selected in the entire energy sector

- **ORGANISATION OF SCIENTIFIC MEETINGS (Selection)**

2022 *Chairperson*: XXII Nat. Congress Div. Ind. Chem. - SCI, 7-8 Nov. 2022 (Catania)

2022 *Chairperson*, CIMTEC 2022, 9th Forum on New Materials, Symposium "Advanced Photocatalytic Materials", Perugia, June 27-29th, 2022, ~100 persons

2019 *Chairperson*, 4th Euro Asia Zeolite Congress, Jan. 27-30th 2019, Taormina, ~150 persons

2018 *Chairperson*, EUROPACAT 2017, 13th European Congress on Catalysis, August 27-31th, 2017, Florence, Italy, ~1400 persons

2015 *Chairperson*, 6th Czech-Italian-Spanish Conference on Molecular Sieves, 14-17th June 2015, Amantea (CS), Italy, ~220 persons

2013 *Chairperson*, 6th IDECAT/ERIC-JCAT Conference on Catalysis, Design advanced multifunctional catalysts for sustainable processes, 3-6th March 2013, Brixen, ~170 persons.

2012 *Chairperson*, 5th International Symposium on Carbon for Catalysis - Carbocat-V, June 28- 30th, 2012 - Bressanone/Brixen, ~160 persons

2007 *Chairperson*, 8th European Workshop on Selective Oxidation (Turku, Finland, 9-30th Aug. 2007), ~170 persons

- **INSTITUTIONAL RESPONSIBILITIES (Selection)**

2022-today Member of the Board of the Industrial Chemistry Division of the Italian Chemical Society

2021- today Coordinator of the Sustainability and Environmental Innovation (SIA) degree course, class L-27, Univ. Messina - Italy, Dept. ChiBioFarAm
2021- today Member of the National Commission for Scientific Evaluation 03 / C2
2019- today Board of Directors of the INSTM Materials Science and Techn. Consortium, Firenze, Italy

- **INTERNATIONALISATION ACTIVITIES AND PROJECTS (Selection)**

2013 – 2020 PI for UNIME of the Europ. Doctorate SINCHEM (Sustainable Industrial Chemistry)
2015-today PI for UNIME of various international collaborations (Univ. di Kuala Lumpur, Malesia and Univ. of Queensland, Australia)
2018 Appointment Committee for Director, Max Planck Inst. for Chem. Energy Conv., Germany
2020 Appointment Committee for Director, ICIQ, Tarragona, Spain
2022 Member evaluation committee Severo Ochoa Centres of Excellence (Ministery of Science)
2021-today Member of the Scientific Advisory Board (ICIQ, Spain)
2016-today Member of the committee of selection of international research projects (EC, ANR – France)
2011-2021 Coordinator of EU projects: INCAS (ID45988, 2010-14), OCEAN (ID767798, 2017-21)
PI in EU projects: TERRA (ID67747, 2015-19), ECO2CO2 (ID 309701, 2012-16), BIOFUR (ID324292, 2013-16), PERFORM (ID 820723, 2019-23), RECODE (ID 768583, 2017-22), A-LEAF (ID732840, 2017-21). *The projects OCEAN, RECODE, ECO2CO2, PERFORM led to the realisation of TRL 5-6 electrocatalytic pilot units*.
2011-2021 Coordinator PRIN2017 (2017WR2LRS), Italy National Projects; PI for UniME in PRIN2015 (2015L5XBSM), PRIN2010-11 (2010A2FSS9), Italy National Projects

Qualification of the Univ. of Messina - UniME (Host Institution) and groups involved in the project

Tradition and change in the centre of the Mediterranean: the University of Messina (www.unime.it) has always been characterised by the quality of research and teaching and by its international vocation. UniME is a generalist university with about 24,600 students, 1,103 teachers and researchers, and is still a point of reference for the entire "area of the Strait". UniME has a positive value (> 1) of economic and financial sustainability, which has been increasing over time, and its ability to attract students, including foreign ones, has also increased. Research funding in Europe drastically increased from 2017 to 2019, with an increase of around 900%.

The University is spread over three locations: a central one divided into several Poles located in different parts of the city and two branches in Noto and Priolo Gargallo (Sicily). It is organised into 12 Departments (www.unime.it/it/departimenti), of which the ChiBioFarAm Department is involved in this project. The ChiBioFarAm Department is located in the Papardo centre (ex. Faculty of Sciences) of UniME.

UniME has an *adequate management structure* inspired by quality criteria and principles of sound financial management: it coordinates and participates in numerous European projects (SCOPE, CRESTING, AMR-TB, ULTIMATE, SOLBIO-REV, DECADE, OCEAN, PEPATO, etc.), projects PON Business and Competitiveness (NI-MOO, GENETIC MARKERS), FESR (SETI, Elettrorigenera, ROTIDOL, etc.), PSR Sicily (CHEESHAL, REM), PON Research and Innovation (AEROMAT, EOLO, BONE ++, etc.) demonstrating the full capacity and quality of sound financial management.

UniME, as a University, primarily combines education and research, as the latter is a prerequisite for providing excellent training at various levels (from the Master to the Doctorate). The Third Mission of the Universities is added to the traditional ones of Didactics and Research. It consists of the enhancement of research and training to generate a positive impact on society by contributing to the development of the territory by enhancing its heritage, proposing new technologies and knowledge, attracting new talents, and stimulating a greater cultural vivacity. This third activity has grown strongly in recent years, thanks to the collaboration with The European House - Ambrosetti.

UniME has a position of excellence compared to other regional and southern Italy universities. It is the first University, among those in the South, for an increase in enrollments in three-year, single-cycle and master's degrees in 2020 (+ 27.4%). UniMe has the highest research productivity among the Universities of the Sicilian Region in terms of citations per researcher (+ 5% and + 8% compared to UniCT and one, year 2020), as well as the highest number of patents among the Universities of the Sicilian Region (+ 100% and + 387% compared to UniPA and UniCT in 2020) and the highest ratio compared to the number of researchers (+ 225% and + 457% as a share of patents per researcher compared to UniPA and UniCT, respectively, the year 2020). The recent update (August 2022) of Stanford Univ. Together with Elsevier (Scopus) on the top2% researchers in all sectors among the over 8.6 M in the world, UniME surpasses the other Sicilian universities (and in the front row among those of the South) both as a number and as their average ranking. *The top-ranked researcher in energy for the South of Italy is part of the group involved in this project*.

The energy and hydrogen sector represents one of the areas of research excellence at UniME. Using the study above by Stanford Univ., about 40-50% of UniME researchers who are among the top 50,000 in the world are from the ChiBioFarAm Department and operate in the sustainable energy sector. The impact of this project on the development of the territory is significant.

Messina, and Sicilia, are one of the areas in Southern Italy with the greatest potential for renewable energy development, but they are severely limited by local consumption capacity. Using renewable energy to produce carriers for energy and hydrogen to facilitate their storage and transport is one of the region's development strategies. There are, therefore, strategic reasons for the development of the proposed activity by UniMe.

The project will mainly involve the **CASPE centre** (Catalysis and sustainable processes) (ww2new.unime.it/catalysis), particularly active in the European field with over 20 European projects and also a reference centre for the INSTM University Consortium on Science and Technology of materials (*www.instm.it*) and the European Research Institute of Catalysis (ERIC aisbl, Brussels; www.eric-aisbl.eu).

The scientific skills available at CASPE are strong and internationally recognised in catalytic processes for energy and green hydrogen. The lab, through ERIC aisbl, is a member of the executive board of the large initiative SUNERGY and derived CSA SUNER-C through a research team member involved in this project. These initiatives aim to develop a large European Action for substituting fossil fuels in energy and chemical production. More than 300 stakeholders are part of this initiative, with many companies in the field. *Thus, this specific project will become part of this large initiative at the EU level, with many benefits regarding visibility, impact on society and company, and industry relations.* CASPE's activities are mainly to developing catalysts and low-carbon footprint catalytic processes for sustainable energy/chemistry and H_2 production.

Operating Units to be involved in the project: the researchers who will be mainly involved are from the ChiBioFarAm Department, particularly the CASPE centre. The CASPE centre comprises 8 professors, three researchers, about 15 post-docs and PhDs in industrial chemistry and chemical engineering, and consolidated collaborations with other scientific sectors at UniMe.

Coordinates the International and Industrial Doctorate ACCESS (Advanced Catalytic proCesses for using renewable Energy SourceS; https://www.unime.it/didattica/post-laurea/dottorati/advanced-catalytic-processes-using-renewable-energy-sources) and is member of the National Doctorates in *i)* Development Sustainable and Climate Change and *ii)* Scientific, Technological and Social Methods Enabling Circular Economy.

The group of Life Cycle Assessment - LCA (prof.sa *Roberta Salomone*, *Dept. Economy*) and of physics of materials for energy (prof.sa *Giovanna D'Angelo, dept. MIFT*) will also participate in the project, as well as other researchers present in the Dept. ChiBioFarAm and of Engineering.

The scientific-technological skills and experience concerning the project idea were described above. The project, in agreement with the call, is presented as single PI activity, but various other very qualified researchers will participate under the coordination of PI (S. Perathoner). In addition to those indicated above, prof. *Gabriele Centi* can be cited (as a member of the CASPE group. He is a well-internationally recognised scientist in catalysis and sustainable processes, with an h-index of 93 and over 35.000 references. He is the President of the world association of catalysis communities and an extensive lecturer worldwide on the aspects closely related to this project, including at the European Parliament. He was part of the team preparing the H_2 roadmap of the MUR and is part of the working group on H_2 of the Sicily region.

In addition, as a consultant, Ing. prof. *Gaetano Iaquaniello* will also participate. He is the former CEO of the NextChem company and is now retired. He has much experience designing and developing industrial plants for H_2 production and their techno-economic assessments. Various papers are in common with the PI. Ing. Iaquaniello and the PI (S. Perathoner) have jointly received the Mario Giacomo Levi Medal of the Italian Chemical Society for the innovative activity carried out in the field of Chemistry that led to industrial implementation. Specifically, this medal was related to the joint activity in developing the waste-to-chemical processes. NextChem has recently received a nearly 200 M€ IPCE grant to construct a waste-to-H_2 plant near Rome. Another is under construction in Venice at Eni biorefinery, and others have been announced.

Since a single PI will present these grants, no partners formally participate in the project. Some of the additional competencies unavailable within the Host Institution will be added through some consultancy (such as the cited Ing. Iaquaniello) and external goods acquired, particularly for manufacturing the prototype unit, which is one of the project deliverables. Although the procurements will follow the requested procedures of the University, it is worth indicating that CASPE already has extensive collaboration with companies such as HYSITECH, with which various pilot units have been made in the framework of various EU projects. *PI has the capability and the network of relations to successfully realise the prototype unit (at TRL5-6) at the core of the SCOOP project.*

The PI, her group and the CASPE centre are involved in various research projects with national and foreign industries, as indicated above. *Thus, there is an extensive network of collaborations with the most relevant research groups in Europe and companies in the project area*. This aspect will also be relevant to achieving the project results, creating visibility for the project, and transferring the results to many different stakeholders to maximise the effectiveness of the impact.

Human resources for the project: the group of the UniME ChiBiofarAm Department specifically involved in this project comprises ~ 25 researchers. It has over 500 m^2 of space for research laboratories in the field of catalysis and sustainable processes for energy and hydrogen. The CASPE centre of UniME has developed or participated in developing various pilot plants in the sustainable energy and hydrogen sector. Four recent EU projects, one also coordinated by the CASPE centre and specifically by PI (S. Perathoner), led to the realisation of pilot units for CO_2 electrocatalytic conversion. Figure 4 reports an example of the pilot unit realised as part of the OCEAN project coordinated by PI. *Thus, human resources and proven capability exist to realise the project objectives.*

CASPE has numerous testing lines for catalysts in flow reactors (including high-throughput) and autoclaves, testing lines for electro- and photo-catalysts and the combination of non-thermal plasma and catalysis. The centre has extensive **i**) analytical instrumentation (various GCxMS, GCxGXxMS, HPLC-MS, IC, AA, etc.), **ii**) equipment for the characterisation of solids (BET, porosity, chemisorption, TPR / TPO, TG-MS, Raman, FTIR, UV-vis reflectance, XRD-EDX) and **iii**) surfaces (XPS, AFM, FTIR with cells to study chemisorption), **iv**) devices for the preparation of catalysts and electrodes also on prototype scale. Some examples of the equipment available to realise the project are presented in Figure 5.

Beneficiary(ies) and other Institutions involved in the project

As indicated above, the grant has to be presented by a single PI together with a Host Institution which in this case are prof. *Siglinda Perathoner* and the University of Messina - Italy (*Università degli Studi di Messina*) having all the characteristics indicated in the advice for the grant (art. 3). Prof. Perathoner is a full professor at the same University. No other beneficiaries and Institutions are involved in the project, but consultants and procurements, as indicated above, will participate in realising the project.

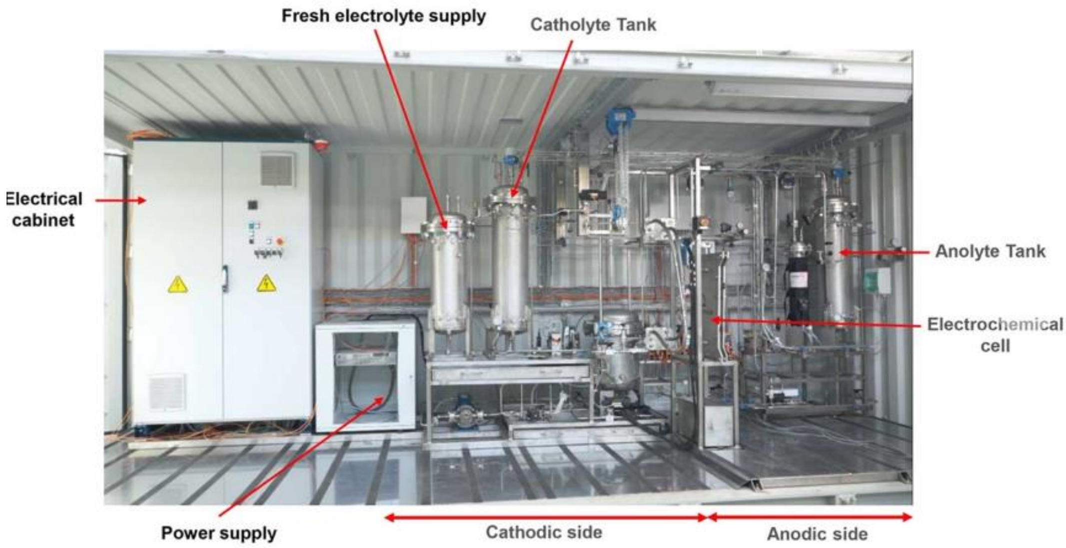


Figure 4 Pilot unit in operation at RWE (Germany) for CO_2 electrocatalytic conversion to FA as part of the OCEAN EU project.

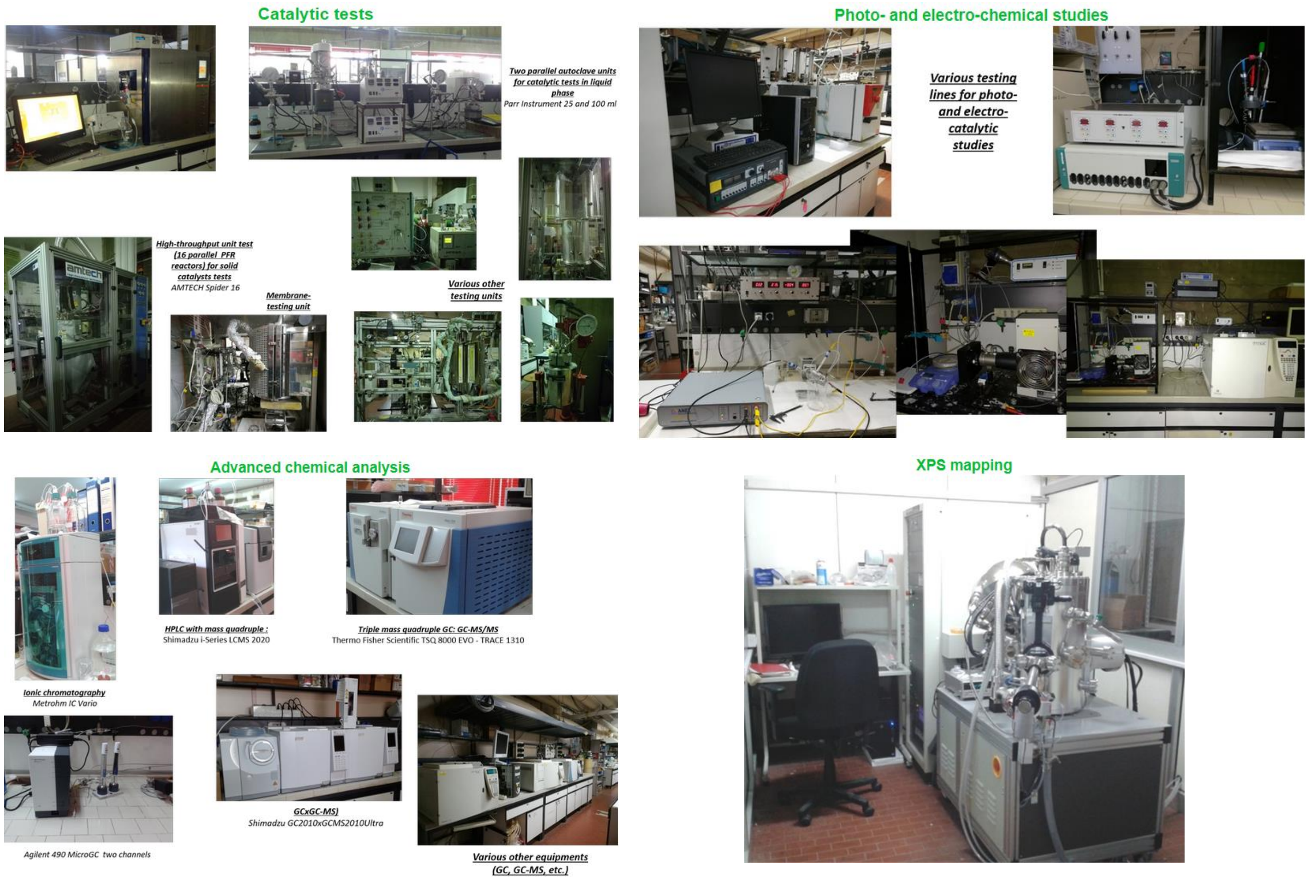


Figure 5 Examples of some of the equipment available at CASPE to realise the project. Further equipment are illustrated at http://ww2new.unime.it/catalysis/equipments.html

The exploitation of the results

As evidenced by the description of PI and the related team, there is *extensive expertise* in collaboration with companies, development of pilot units, and an extensive network of international collaboration with many stakeholders and companies. Among some of the companies in the field of potential interest for the project results having already collaborations or interactions with PI and team are Versalis, Casale, Avantium, Siemens Energy, Engie, Total, Hysitech, Motor Oil, RWE, Toyota, Shell, NextChem, Snam, A2A, etc. *Thus, the proven capability exists to develop the proposed technology up to TRL 5-6 and then use the results to identify companies to exploit the results.*

Autonomy and decision-making capacity

As the CV outlines, the PI has coordinated or was the PI for the UniME research unit in many EU industrial and national projects. A selection is reported in the following:

- PRIN 2017: CO_2 as the only source of carbons for monomers and polymers: a step forward circular economy (CO_2 ONLY), *National Scientific Coordinator*
- H2020-767798: Oxalic acid from CO_2 using Electrochemistry At demonstratioN scale (OCEAN), ongoing, 48th months, *Coordinator of the project*
- FP7-NMP2-LA-2010-245988 Integration of Nanoreactor and multisite CAtalysis for a Sustainable chemical production (INCAS), 48th months, *Coordinator of the project*
- FP7-2012- 309701: Eco-friendly biorefinery fine chemicals from CO_2 photo-catalytic reduction (ECO2CO2), 36th months, *Scientific responsible for UdR ME*
- Industrial Project with ALTA, *responsible*
- Industrial Project with TOYOTA, *responsible*
- FETPROACT-2016, An Artificial Leaf: a photo-electro-catalytic cell from earth-abundant materials for sustainable solar production of CO2-based chemicals and fuels (A-LEAF) "Project ID: 732840, *scientific responsible for UdR ME*
- IAPP CONTRACT 324292-2013. BIOFUR: BIOpolymers and BIOfuels from FURan based building blocks. A Marie Curie Industry-Academia Partnerships and Pathways, 36th months, *Scientific responsible for UdR ME*
- H2020-NMBP-ST-IND-2018-2020, PowerPlatform: Establishment of platform infrastructure for highly selective electrochemical conversions (PERFORM), project 820723, *Scientific responsible UdR ME*

There is thus a well-proven autonomy and decision-making capacity of the PI.

The organisation of the activities and coordination by PI (with other participating partners)

Being the grant presented by a single PI and a Host Institution (UniME), there are no issues of organisation and coordination of the activities of other partners. The largest part of the project will be done by the team already coordinated by PI and well internally structured in terms of competencies and sub-teams. To the project, a limited number of additional groups of UniME will participate: Prof.sa D'Angelo (Dept. MIFT) is competent in solids' solid and surface physics and prof.Sa Salomone (Dept. Economy) has expertise in LCA. There are already consolidated relations between them. Ing. Iaquaniello, external to UniME, will participate as a consultant for the aspects related to the techno-economic evaluation of the project. With Ing. Iaquaniello, there has been a long-term and extensive collaboration. An external company should manufacture the prototype. Thus, all participants not involved in the CASPE laboratory, directed by PI and the main UniME centre involved in executing the project, have well-defined activities and have already established collaborations. *Thus, there are no problems with organisation and coordinating the project by PI.*

A person not directly involved in the project and research activities (prof. G. Centi) will be responsible for the *quality and monitoring of the project*, reporting directly to PI for any issues and deviations. A committee formed by Group Leaders (senior researchers) will also assist PI in monitoring the project and coordinating the scientific and reporting activities.

SECTION 2

Description of the research proposal

SCOOP focuses on increasing from TRL 3 to TRL 5-6, a solar-driven (artificial-leaf-type) device for the continuous (24h) production of green H_2 from water. The device is composed of an electrocatalytic (EC) cell coupled to a photovoltaic (PV) module, with the PV-driven EC cell able to convert CO_2 and water to a mixture of H_2 and formic acid (FA). The latter is an intermediate storage chemical used to generate H_2 during dark periods, forming back CO_2, which can be recirculated. The concept was schematically presented in Figure 1.

The starting TRL 3 derives from a previous EU project (A-LEAF, ID#732840, ended 6/2021), where the UniME group developed and engineered an artificial-leaf-type cell up to TRL 3, where CO_2 and water were converted to formic acid (FA) using sunlight. The electrodes of this cell were based on earth-abundant materials without applying any external bias or use of sacrificial agents. The cell design and operation (electrolytes, etc.) were also suitable for scaling up and industrial exploitability. World-record results were obtained in this cell, as commented in the synopsis and presented in Figure 2. Still, the A-LEAF project focused on converting CO_2 to FA rather than using FA as an intermediate storage element to realise continuous H_2 production. Thus, the SCOOP project starts from the A-LEAF TRL 3 results but gives a new applicative perspective.

SCOOP will do (**1**) non-predominant *fundamental research* to optimise electrodes and cell design to enhance further STF, stability and productivity; (**2**) *prevailing industrial research* for **2.a**) scaling up to TRL 5-6 the cell, **2.b**) testing its stability, **2.c**) integrating the unit to decompose FA catalytically during dark periods to have a continuous (24h) production of H_2, **2.d**) Design, manufacture and operate the prototype, **2.e**) evaluate the techno-economic costs of H_2 production, and assess the impact by LCA; (**3**) non-predominant *experimental development* to create a *Solar Fuel Hub* to showcase the results to stakeholders and the public.

The general Pert chart of the SCOOP project is presented in Figure 6.

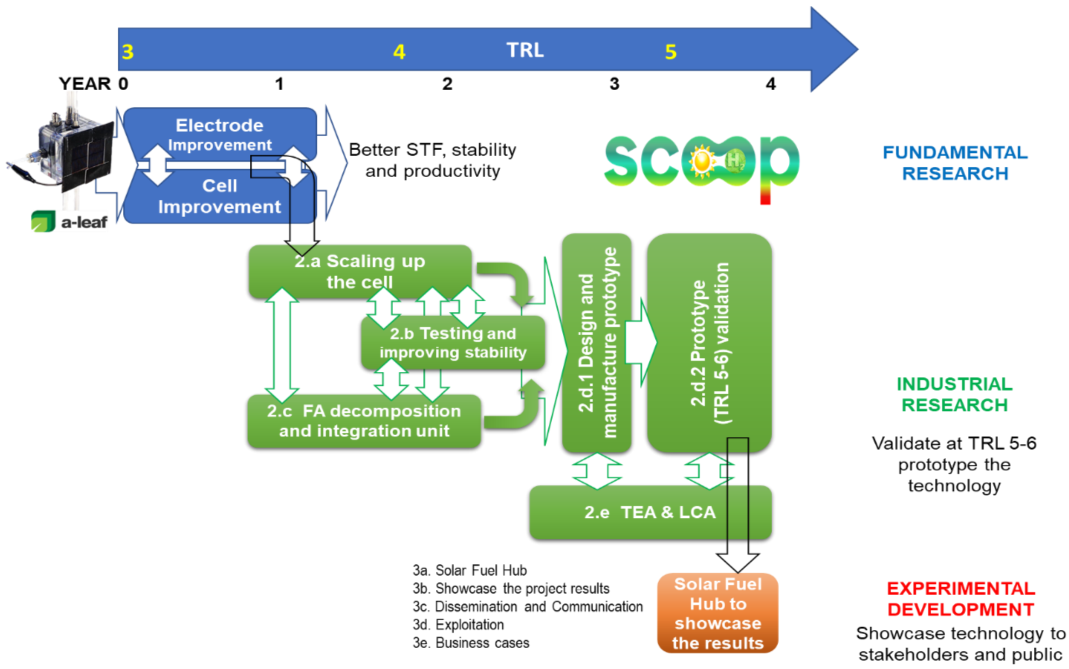


Figure 6 Pert chart of the SCOOP project, indicating the main actions and their timing and contribution to increasing the TRL, organisation in terms of typology of research and their aim, and main interactions between the activities.

Description of Fundamental Research Activities

The SCOOP project's fundamental research is dedicated to optimising electrodes and cell design to further enhance STF, stability, and productivity. It is a non-predominant but critical element of the projects. The aim is an experimental work to improve and optimise the critical elements of the proposed technology from a fundamental perspective, e.g., the electrocatalysts, electrodes, and cells. The starting point is the PoC of one central element of the proposed novel process scheme, summarised in Figure 1. It is the PV-EC artificial-leaf type device developed earlier up to TRL 3 as part of the ended EU FET project A-LEAF.

Starting TRL 3 level

The starting element is the cell and electrodes developed up to TRL 3 (proof-of-the-concept, **PoC**), which is limited to the PV-EC cell to produce H_2+FA from CO_2 as part of the cited A-LEAF EU project. Figures 2 and 7 show this cell.

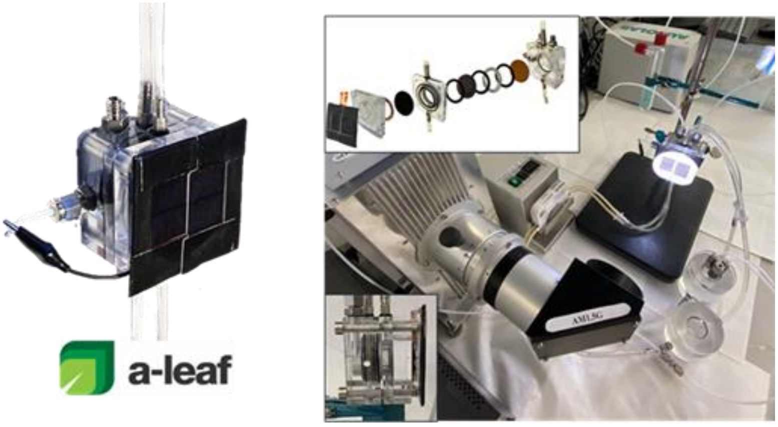


Figure 7 Solar-to-fuel A-LEAF PV-EC. The lab-scale prototype consists of a high-compact electrochemical cell (EC) coupled with a Photovoltaic (PV) module (4 cells encapsulated in glass). A solar simulator is integrated into the platform for standard solar irradiation (1 SUN).

The size of the PV and electrode was around 8-10 cm^2. It was a small-scale lab-scale prototype for the PoC. The electrodes are based on earth-abundant materials, while most literature data use noble metals and other critical raw materials as electrocatalysts. Furthermore, STFs have often been reported only for quite low current densities and even so, STFs lower than about 5% have been reported, as presented in Figure 2b. In addition, the reactors and operative conditions often do not allow operations and industrial scalability robustness.

The results of the previous A-LEAF project, which will be the *starting point* for the SCOOP project, are **i**) combined η_{STF} (STP efficiency) of ~6-7%) at a current density > 15 $mA \cdot cm^{-2}$ in converting CO_2 into HCOOH (FA), **ii**) cell design based on gas-diffusion-electrodes (GDEs) with integrated PV module (see Fig.s 2, 7), **iii**) electrocatalysts/electrodes based on earth-abundant elements. This lab-scale artificial-leaf-type (AL) device has a compact design (suitable for scale-up) and uses advanced GDE based on Cu-S for CO_2 reduction and Ni-Fe-Zn oxide for water oxidation. These electrodes' Faradaic efficiency (FE) was around 60% to FA, while the remaining is H_2, with only traces of CO.

Planned activities to increase TRL

Obtaining a combined FA + H_2 is an objective of the SCOOP project, but the side formation of CO, even if in low amounts, should be avoided. One objective of electrode and cell improvements in fundamental research activities is thus to eliminate side CO formation and optimise the FA to H_2 ratio to the optimal value to the scheme of production outlined in Figure 1. Furthermore, tests of the electrodes in the A-LEAF project were up to about 20 hours on stream (the cell operates in a continuous mode). The stability of the performances has to be extended to at least 100h without significant deactivation (less than 5-10% of the initial value). SFT and productivity (current density) also have to be further improved.

These are thus the <u>objectives</u> for the fundamental activities part of the SCOOP project:

i) Reduce the formation of CO as a byproduct below ten ppm;

ii) Increase the current density to over 20 $mA \cdot cm^{-2}$;
iii) Increase the stability of the performances (less than 5% lowering of the current density in tests for at least 30h of time-on-stream).

These objectives, which are planned from M1 to M15, as indicated in the Pert chart (Fig. 6), are reached through two main activities:

1. **Activity 1a**: Electrode Improvement.
2. **Activity 1b**: Cell Improvement.

These activities are planned to increase the TRL to nearly a TRL 4 value.

1a. Electrode Improvement

It relates to the synthesis, characterisation and testing of modified electrocatalysts/electrodes for the anodic and cathodic parts of the EC cell. The synthesis procedure and composition will be tuned to enhance the performances (Faradaic selectivity, current density, stability) to reach the target objectives, starting from the materials developed in the frame of the previous project. The plan of activities includes:

i. The synthesis and modification of the electrocatalysts starting from the initial Cu-S for CO_2 reduction and Ni-Fe-Zn oxide for water oxidation; it is planned to prepare at least 5 electrocatalysts for the anodic part and 5 electrocatalysts for the cathodic part, taking into account also the latest literature results; the synthesis methodology to prepare these electrocatalysts will consider in particular the following aspects: a) avoid the use of critical and/or expensive raw materials; b) use non-toxic substances and not leading to toxic waste; c) use a procedure which can be scale-up industrially.
ii. The characterisation of these electrocatalysts using a combination of physico-chemical techniques available within CASPE laboratory, in particular AA, XRD, Raman and FTIR, UV-Visible in reflectance, porosity and surface area, XPS, SEM, etc.
iii. Preparation of the electrodes from the electrocatalysts. In particular, GDL-type (gas-diffusion layer) for the electrodes for CO_2 reduction. Electrodes with size in the 5-10 cm^{-2} range will be prepared and then joined to a proton-conducting membrane such as Nafion to form the membrane electrode assembly (MEA) composed of the membrane on which faces are the anodic and cathodic electrodes.
iv. Perform electrochemical tests (cyclic voltammetry, electrochemical impedance spectroscopy - EIS) to study the electrodes and the presence of limiting resistances to their performances from an electrochemical viewpoint. Provide feedback to optimise the preparation.
v. Tests the MEAs (see activity 1b) and then characterises the electrode after the tests to analyse possible changes in their characteristics and composition occurring during experiments.

Electrode optimisation: The anode and cathode from the original A-LEAF design will be further optimised in two main directions:

1- *Chemical modification*: The catalyst performance will be fine-tuned with additional doping with earth-abundant elements (Al, Bi, S, Mn, Zn);
2- *Nano-structuration* (e.g., nano-islands of Cu or other elements on porous nanocarbon supports or single-atom electrocatalysts with fine-tuned nanoarchitecture).

The interface and size of the catalysts on the electrodes will be further optimised by modification in the processing protocols (thermal and chemical). Alternative electrode supports beyond carbon GDLs, such as metal diffusion electrodes, will also be explored, which may improve electrical conductivity in the MEA, to minimise its drop.

Characterisation and stability: The new electrodes will be characterised with electrochemical protocols in a 3-electrode system by CV, LSV, chronopotentiometry (CP) and also electrochemical impedance spectroscopy (EIS) to analyse the improvement, or not, of the proposed modifications. A pass/no pass list of requirements will be indicated to decide which electrodes meet the requirements for full-cell implementation. In the case of CO_2 reduction, in addition to electrochemical performance, the electrodes will be benchmarked as a function of CO_2 purity/ratio in the gas feed as another relevant parameter.

It is planned that about 18 PMs (person-months) among structured and project-hired researchers will be necessary to perform these activities.

1b. Cell Improvement

It relates to the a) optimisation and engineering of the PV-EC cell to minimise further the resistance and enhance the performances and productivity, b) testing and ranking the materials developed in activity 1a, providing feedback on their behaviour.

Optimise cell design: The original A-LEAF cell design will be further optimised to meet project targets in two main directions:

1. Investigation of *physicochemical factors* (resistances, interfaces, transfer processes, etc.) and materials (electrode & membrane characteristics, electrolyte) limiting the performances;
2. *Cell engineering*; flow distribution and micro-fluid dynamics, bubble formation and sticking to the electrolyte, the connection between EC and PV elements, minimisation of resistance and losses, minimisation of dead volume and electrolyte, optimal GDL characteristics The scheme of the optimise cell design is presented in Fig. 8. It shows a cell design facilitating scale-up and industrialisation; the cell engineering, also using suitable simulation tools, will allow minimising losses in efficiency based on the dedicated studies to determine critical factors.

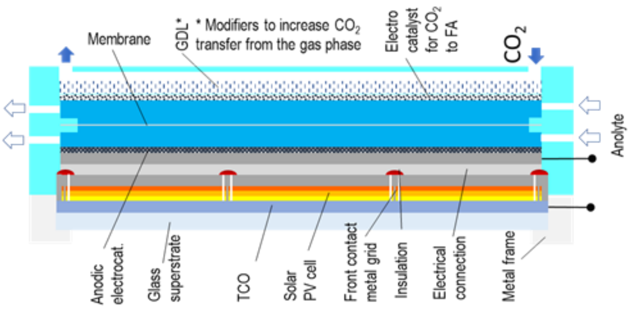


Figure 8. Schematic preliminary design of the PEC prototype cell.

A series of experiments will also be dedicated to analysing the purity level necessary for CO_2 inlet feed and the influence on the performance of recycling CO_2 after FA decomposition. In collaboration with external research centres (especially Forschungszentrum Julich GMBH; a long collaboration has been established with them), the optimal PV module will be identified with the appropriate potential and current density. Aspects considered will include:

Optimal active area ratio. This activity will analyse the impact of the active area ratio on coupling and solar-to-fuel efficiency (STF) in lab-scale PV-EC prototypes. Low-cost silicon heterojunction modules (shingled interconnected) with variable output characteristics will drive the PV-EC device. The photovoltaic (PV) modules will target an efficiency of 21 %. The PV modules for integration with the EC cell will contain 4 or 5 serially connected SHJ cells to provide a maximum power point voltage in the 2.0 – 3.0 V range. The actual number of cells (4 - 5 or more) in shingled will be defined by the V(J) characteristics of the electrochemical cell (EC). Analysis of the active area ratio of PV and EC components using the polarisation curve of the catalyst system will be used to achieve the best coupling and maximise the STF efficiency.

Manufacturing of optimised PV module. This will be made externally to UniME through procurement. A Shingled silicon heterojunction (SHJ) module with optimised PV parameters for integration with the EC component of the prototype will be manufactured after analysing the optimal design for integration with the EC unit to minimise loss of solar conversion efficiency due to edge effects. Shingled solar modules are prepared by laser cutting the silicon heterojunction silicon solar cells into stripes (shingles) that are assembled in strings by connecting the front of a shingle to the back of the next one, typically using Electrically Conductive Adhesive (ECA). Figure 9 shows the J-V (current-voltage) characteristic, photovoltaic parameters, and photograph of a shingled mini-module of 5 connected in series SHJ solar cells.

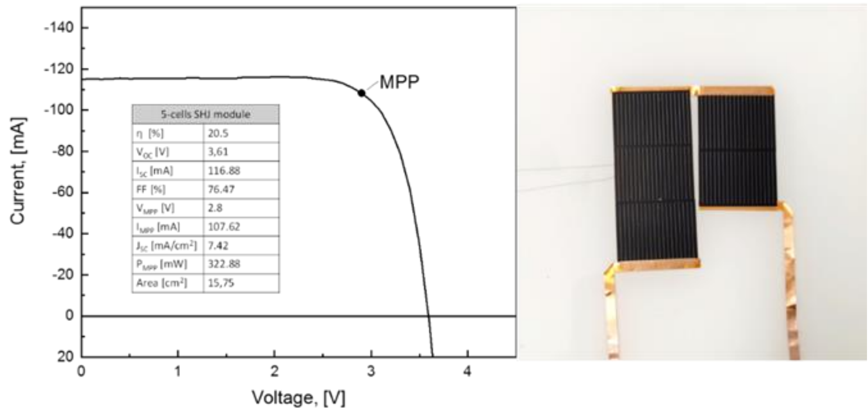


Figure 9. J-V characteristic, photovoltaic parameters, and photograph of a shingled mini-module of 5 connected in series SHJ solar cells. Courtesy of partner Jülich from which the cells will be procured.

The optimal cell configuration and related electrodes will be further analysed regarding scalability, optimal PV characteristics, and integration within the cell. The lab-scale cell (5-10 cm^2 electrode size, flow continuous operations) will also be used to test and rank the new electrodes prepared. Feedback in terms of electrode characteristics for their optimisation will also be given. An example of the cell that will be used in these lab-scale developments is presented in Figure 10, reporting a 3D modelling of the different components forming the EC and a photo of a homemade flow cell in Plexiglas to allow visual inspection. The thickness of the two liquid chambers is very low to minimize overpotential due to the presence of electrolytes between the two electrodes. The use of silicon gaskets guarantees the sealing of the reactor. The lab-scale prototype will be carefully validated after the fabrication and assembly of all the parts. All the leaks must be eliminated for a good tight of the cell, and the electric contacts, especially with the GDL, must be optimized.

This cell will be used to optimize the lab-scale EC cell, conduct experiments on anodes and cathodes developed in 1a activities, and verify the cell design for the construction of the scaled-up prototype.

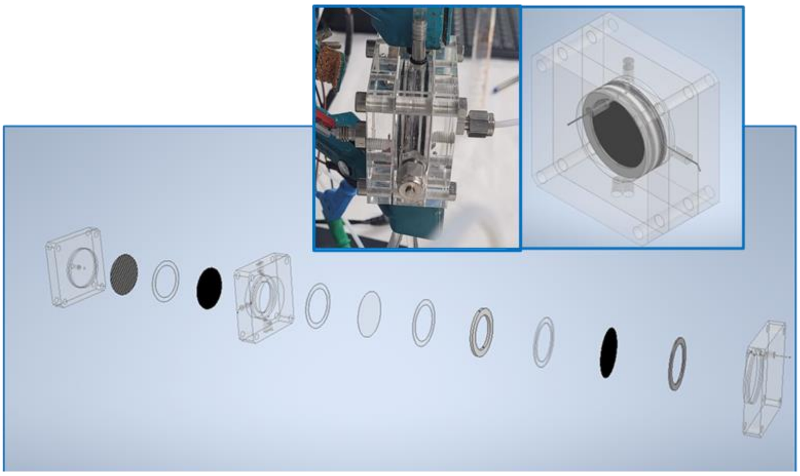


Figure 10. 3D model of the lab-scale flow-through EC device, including all the components (electrodes, silicon gaskets, etc.). The photo reports a side picture of a flow-through EC reactor.

It is planned that about 18 PMs (person-months) among structured and project-hired researchers will be necessary to perform these activities.

Description of Industrial Research Activities

This is the predominant part of the projects' activities and aims to increase TRL to 5-6. The planned research aims to acquire knowledge and skills to develop the novel process scheme under study. The focus is on **i**) the activities for the scale-up of the technology up to TRL 5-6, **ii**) the investigation of the other process components to complete it (in particular, the step of FE decomposition), **iii**) the validation of the technology in the whole and regarding the stability of the operations, and **iv**) demonstration of the environmental and techno-economic feasibility.

The step of FA decomposition is considered, from literature results, at TRL 3.[11-13] It is *not* considered an element for which dedicated fundamental research would be necessary. Therefore, the research will be only part of the Industrial Research activities and will focus on integrating this step into the whole process scheme (Fig. 1). The decomposition of FA will be made directly in the aqueous solution obtained by recovering FA from the AL-type continuous cell. Solid-type catalysts and supported Pd bimetallic catalysts[12, 13] will be used for the study.

As a key element for TRL 5-6, this industrial research includes the construction of a prototype operating in a laboratory environment. The electrode size considered generally valid for such a type of experimentation is 10-15 x 10-15 cm (an increasing factor of about 30 to the lab-scale reactor), with a preliminary design illustrated in Figure 8 for the AL-type section. It will then be integrated with the other components for H_2/FA separation, FA decomposition and recycling of CO_2. The prototype will be used for the validation of the technology, the tests on continuous operations and stability performances, and as a showcase for the technology.

The activities planned for the Industrial Research part of the project are the following:

- 2.a scaling up to TRL 5-6 the cell;
- 2.b testing and stability;
- 2.c integrating the unit to decompose FA catalytically during dark periods to have a continuous (24h) production of H_2;
- 2.d Design, manufacture and operate the prototype
- 2.e evaluate the techno-economic costs of H_2 production, and assess the impact of LCA.

A preliminary isometric view of the test bench, with (on the left) an exploded view of the cell for the prototype testing unit, is shown in Figure 11.

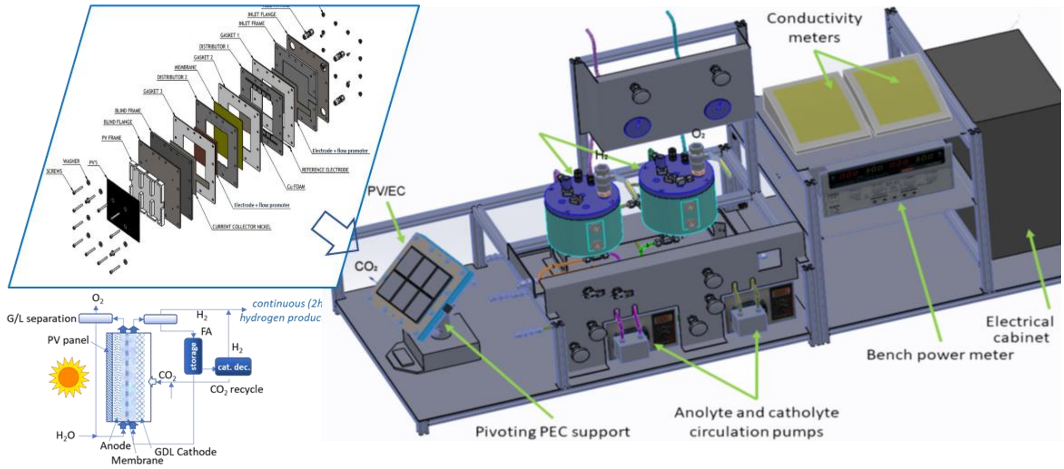


Figure 11. Preliminary isometric view of the test bench. On the left, an exploded view of the cell.

The test bench is designed to be used as desktop equipment. The first draft of the design is reported in Figure 11. The rig will have an aluminium frame, and the footprint of the equipment will be 500 × 1000 mm. The test rig is split into 4 areas:

1. PV/EC area: here, the PV/EC device is installed on the pivoting support, allowing it to be oriented towards the sunlight. The possibility of installing it on a sun tracker is under investigation. This way, the PV/EC cell will automatically be oriented towards the sun.
2. Process area: the pumps, vessels and all the fluid management systems are in this section.

3. Analytical area: the instrumentation used to monitor the process conditions will be installed in this section i.e., conductivity and temperature, bench multimeter, etc.
4. Electrical cabinet: the power will be connected to the electrical that will distribute it to the rest of the equipment and will also include any protection (i.e., fuses and/or magneto-thermal and differential switches)

The tubing, valves and wetted equipment will be chosen according to the chemical compatibility with the substances in the system. Hence, most of the equipment will have plastic materials for the parts wetted by the electrolyte to ensure chemical compatibility (e.g., PTFE, PP and Tygon). The PEC device and the PEC test rig have been designed according to the engineering specifications, and P&ID gathered from the previous activities.

The TRL 5 PV/EC will have a 10-15 x 10-15 cm cell mounted on a rack to allow transport to the other locations to demonstrate the technology. Sampling points on the PV/EC reactor outlets and liquid and gas streams will be foreseen to collect samples or connect analytical equipment to evaluate composition and production rates, rate of H_2 production, cell performance, stability, etc. The photocurrent and potential generated by the PV will be monitored as well.

The test bench will be designed with two symmetrical liquid loops feeding the PV/EC device and also acting as the gas/liquid separation elements to recover H_2 and O_2 (see Fig. 1). Two additional vessels will act as the intermediate storage for FA and for its catalytic decomposition to produce H_2 and CO_2 which is recirculated. Peristaltic pumps, controlled by a computer unit with dedicated software, will regulate and monitor the overall device. At the inlets of the cell, two rotameters are placed to measure and monitor the flow rates. This allows regulation and minimization of the cross-membrane pressure difference. The catholyte and anolyte vessels have a total volume of 1000 mL. The conductivity and temperature of the electrolyte are measured using two multiparameter instruments. Finally, the carbon dioxide (including them recirculated) is fed on the EC through a gas-diffusion-layer (GDL) cathode. The P&ID of the test bench will be used to optimize this preliminary design and verify safety aspects through HAZOP and derived methods. Safety equipments to control emissions and critical components will allow safe operations.

Timing and relations between the tasks and with Fundamental Research and Experimental Development activities are outlined in Figure 6 (Pert chart), together with the indication of how they contribute to the increase in TRL. Procurements will be used to manufacture the PV module and prototype, as these competencies within UniME are unavailable. However, experience exists in external collaboration on these aspects in the frame of other pilot units realised in other projects. A consultant with wide experience in these aspects will be used for the techno-economic engineering assessment. Instead, internal competencies in UniME (but other dept.) will be used for the LCA.

2a. Scaling up the cell.

This activity is planned from M13 to M27, see Figure 6, with an increase in TRL up to 4-5. It is a preliminary activity before the design and manufacture of the prototype. The main elements of this activity are:

i) Scaling up the preparation procedure of the electrocatalysts and electrodes to **a**) prepare larger, uniform, and well-reproducible electrodes, **b**) use methodologies suitable for further scaling-up and industrial realisation of the electrodes.
ii) Scaling up and optimisation in terms of minimisation of the internal resistances, increase robustness and decrease the costs of construction of the AL-type cells, including the integrated PV module.
iii) Engineering design of the cell and electrode-membrane assembly to optimise the fluxes and the uniform distribution across the entire electrode, also avoiding effects such as bubble sticking, which may lower performance.

The optimum electrodes reaching the expected targets will be further scaled up to the required dimensions. This may imply small modifications in the processing protocols. The most convenient protocols will be selected, and the electrodes with the desired size, resistance, and catalytic performance will be fabricated at prototype dimensions to construct the prototype. The optimal cell configuration will be further analysed regarding scalability and cell design. A CAD design for the cell will then be developed, with the identification of the optimal PV characteristics for cell integration.

For the PV module integration, the active area ratio of PV and EC components will be analysed using the polarisation curve of the catalyst system to achieve the best coupling and maximise the solar-to-fuel efficiency of the prototype.

It is planned that about 23 PMs (person-months) among structured and project-hired researchers will be necessary to perform these activities.

2b. Testing and stability.

This activity is planned from M18 to M33, see Figure 6, with an increase in TRL up to 4-5. It is a preliminary activity before the design and manufacture of the prototype. The main elements of this activity are:

i) *Testing:* **a**) tests the electrocatalysts/electrode developed in 2a. in the optimised lab-scale system, **b**) ranks them against the target performances with feedback to the preparation.

ii) *Validation of the scalability*: **a**) analyse the deviation in the performances during the scale-up of the preparation, **b**) analyse eventual deviations in electrode performances during the scaling-up procedure, **c**) identify their reasons and the necessary modifications to the electrode or cell design to minimise them. For this last sub-activity, the samples will be characterised by the combination of physicochemical and electrochemical methods mentioned before to determine changes in the electrocatalyst and/or electrode which cause the variation in performance.

iii) *Stability***: a**) initial evaluation of the stability with feedback on the preparation, **b**) analysis of the sensitivity of the performances to quality of CO_2 and water feed, and possible impurities. If signs of deactivation are identified, the deactivation mechanism will be investigated. The starting point will be the characterisation of the samples by the combination of physicochemical and electrochemical methods mentioned before after the stability tests. Accelerate deactivation procedures will also be identified to have a complete evaluation of stability and possible issues.

It is planned that about 21 PMs (person-months) among structured and project-hired researchers will be necessary to perform these activities.

2c. FA decomposition and integration of this unit within the process scheme.

This activity is planned from M13 to M27, see Figure 6, with an increase in TRL up to 4-5. This activity focuses on these aspects:

i) Selection of the suitable solid catalysts for the FA decomposition module. Based on the literature, the starting catalyst will be 5% Pd/AC (active carbon), used as pellets (1-2 mm size) in a fixed bed reactor through which the FA solution (recovered from the Al-type unit) passes. The catalyst will be optimised by adding dopants and creating an alloy with a second metal. Alternative non-noble metals such as Ni will also be tested.
ii) Optimisation of the performances, particularly on-off operations, to allow the production of H_2 on demand.
iii) Analysis of the effect of the impurities present in the FA stream from the AL-type reactor.
iv) Engineering evaluation of the integration of this unit in the process scheme (Fig. 1) to allow a continuous (24h) production of H_2.

It is planned that about 25 PMs (person-months) among structured and project-hired researchers will be necessary to perform these activities.

2d.1 Design and manufacture of the prototype.

This activity is planned from M30 to M36, see Figure 6, with an increase in TRL to about 5. As indicated before, the prototype (see Fig. 11) will have a size of the characterising elements (PV module, electrodes for the EC cell) around 30 times higher than the lab-scale device (Fig. 10) used in the initial experimentation. The scaling-up of these devices is largely based on numbering (e.g. in a series of parallel units) rather than in terms of the size of the unit itself. This scaling factor for electrocatalytic-type devices is thus typically considered valid for the target TRL.

The prototype will also include the other elements in the process scheme presented in Figure 1 (different from the lab-scale unit) and the controlling elements to allow continuous operations to demonstrate feasibility. The prototype will be on a skid to allow its transport and location at different places. The manufacturing of the prototype and the PV module will be realised using external resources (procurement), being not possible within the workshop capabilities of UniME.

This activity focuses on these aspects:

i) *Engineering design and safety*. Based on the inputs of the previous activities, the prototype design specifications to prepare the Process Flow Diagram (PFD) and Piping and Instrumentation Diagram (P&ID), containing all the elements (connections, valves, controls, pumps, etc.), the inputs and outputs that have to be controlled, and at which interfaces. This draft P&ID, together will all information regarding the chemicals used, the process conditions, the mass flows etc. (PFDs), will be the input of a hazard and operability study (HAZOP). This will be a structured examination of the planned technology platform to identify and evaluate problems representing personnel, equipment, or operations risks. The outcomes of the HAZOP will have to be implemented in the planned design to ensure safe operation. These outcomes will be used to make a final P&ID. The final P&ID will list all necessary piping and instrumentation for the skid prototype unit and related safety, control and analytical components.

ii) *Development and building*. Based on the design, PFD and P&ID, the skid prototype unit (construction work, assembly of components and installation of auxiliary equipment including piping, gas supply, electrical works, sensors, etc.) will be assembled. The task includes the fabrication and/or the assembling of components and structures, including all the equipment, the piping systems, the mechanical systems and the electrical systems required for the plant's construction. All structures for supporting the equipment and its piping and the tubing for instrument connection to process (i.e. gas analyser tubing, pressure measurements, etc.) will be fabricated and tested. Sub-units supplied by partners, electrical systems (i.e., controllers and equipment), and the electrical and signal distribution (i.e. cable trays, wiring, etc.) will be assembled/installed. A software interface will allow operators in the control room to monitor and acknowledge the status of each unit, and users will have information on the plant's operational parameters. The remote interface will allow monitoring and, when authorised, to interact with the plant units. After every unit's mechanical completion and due testing, the prototype unit will be located at the *Solar Fuel Hub* for the planned testing and stability campaigns under environmentally relevant conditions (TRL 5-6) and as a *showcase* for stakeholders and the public.

The prototype will be designed as a working unit, thus with all the necessary elements for continuous operations and testing.

It is planned that about 13 PMs (person-months) among structured and project-hired researchers will be necessary to perform these activities and use the cited external resources.

2d.2 Prototype validation.

This activity is planned from M37 to M48, see Figure 6, with an increase in TRL to about 5-6. The prototype, after the necessary preliminary mechanical testing and safety assessment, will be used to validate the performances under environmentally relevant conditions (TRL 5-6):

a. the electrodes prepared, providing feedback for eventual improvement,
b. prototype performances (concerning project targets and eventual deviations to lab-scale devices, providing feedback for eventual improvement in the design)

c. stability (≥100-200h) with simulated and/or real streams and illumination.

The testing will include the *quantification* of the following aspects:

- the **1**) solar-to-fuel efficiency, **2**) the current density, **3**) the rate of H_2 and FA production, and **4**) the quality of H_2 produced (presence and type of eventual other components) obtained during operations in the presence of solar (or simulated) illumination;
- the **5**) rate of production of H_2, and **6**) quality of hydrogen produced during operations in dark conditions;
- the stability of the operations, **7**) during illuminations, and **8**) during dark conditions; the effect of **9**) multiple cycles between illumination and dark conditions
- the requirements in terms of **10**) the quality of the feed (water, CO_2) and **11**) the possibility of using water and CO_2 obtained by condensation from the air;
- the data for **12**) a refinement of the technology's cost analysis and life-cycle assessment.
- the assessment of **13**) the reliability and robustness of operations,
- the flexibility in providing **14**) an *on-demand* supply of H_2 for residential, agricultural or energy community applications.

The results will provide eventual feedback to the other activities to improve further the technology.
It is planned that about 30 PMs (person-months) among structured and project-hired researchers will be necessary to perform these activities.

2e. Techno-economic and life-cycle assessments (TEA & LCA).

This activity is planned from M30 to M48, see Figure 6, with an increase in TRL to about 5-6. The results of both lab-scale and prototype units will be used for TEA and LCA assessment of the technology using internal and external resources as described before.

- *Techno-economic and engineering assessment.* This activity will be focused on the technical and economic assessment of the PV+EC unit for the continuous (or on-demand) process of H_2 production. A detailed flowsheet of the overall process will be developed for the selected case studies (continuous or on-demand cases). The relevant operating parameters will be identified and used to perform a sensitivity analysis to define an optimised configuration and assess production costs. The input data will initially be those obtained in the lab-scale unit and then progressively updated with the data obtained from the prototype unit.
  A Basic Engineering Design comprising the preparation of a Process Flow Diagram (PFD), Heat and Material Balance (H&MB), Process Data Sheet (PDS), Utility consumption list (UCL), Piping&Instrument Diagram (P&ID), operational and control philosophy as well as a proper strategy to manage the intermittence of solar energy source will be developed. Data collected in Basic Engineering Package will be used for economic analysis.
  CAPEX and OPEX will be evaluated up to the final cost of production (COP) of H_2 in the two considered application cases. A detailed techno-economic feasibility model will be developed to check the economic feasibility under different scenarios. These activities will be made mainly through the use of an external consultant.

- *LCA and environmental impact*. Environmental impacts and cost of the process will be evaluated from a simplified life cycle point of view. The simplified LCA study will be conducted following ISO standards 14040 and 14044 and entail (i) scope and boundary definition, (ii) gathering of life cycle inventory, (iii) life cycle impact assessment and (iv) interpretation. It will be carried out iteratively to assist the technology development throughout the project. The techno-economic engineering assessment will acquire the mass and energy input-output data. The life cycle impact assessment will focus on energy efficiency, cumulative energy demand and global climate change indicators. These indicators will be used to assess whether energy efficiency and CO_2 emission targets are met from a holistic point of view. In addition to these indicators, environmental gains or avoided burdens created by the production of green hydrogen will be investigated with a range of life cycle impact indicators. The results will be compared against the production of H_2 using the

combination of PV + electrolysers (without external H_2 storage) and conventional or alternative productions of H_2 (including storage and transport, eventually using hydrogen vectors).
The contribution of this hydrogen production technology to the circular economy will be evaluated with a material circularity indicator (MCI).

It is planned that about 12 PMs (person-months) among structured and project-hired researchers will be necessary to perform these activities in addition to external consultants.

Description of the Experimental Development Activities

This is a non-predominant part of the projects' activities and aims to increase TRL to 5-6. These activities aim to acquire, combine, structure and use the scientific, technological, and other knowledge and skills developed with the project to **i**) showcase the technology to stakeholders and the public, identifying as a side aspect also the possibilities of acquiring resources and skills for the further development of the technology, and **ii**) perform a preliminary analysis of the exploitability and market perspectives, also based on the analysis of the business cases. The result will be the definition of an exploitation strategy for the proposed technology.

The experimental design is based on the prototype and related results developed with the Industrial Research activities. A central aspect of these technologies is the creation of a *Solar Fuel Hub*, having as the mission to **a**) showcase the results to the public and perform actions of dissemination and communication for different targets (the scientific community, companies and other stakeholders, and the public and society), and **b**) analyse the exploitability of the technologies and its market perspectives, defining eventually one or more business cases and especially an exploitation plan.

Although the core of these activities is planned for the last year of the project (M37-M48), e.g. when the at least initial results of the prototype are available (see Pert chart in *Figure 6*), some of the dissemination and communication activities will start earlier.

The Experimental Development activities are the following:

3a. Creation and Operation of the Solar Fuel Hub

It will be created at UniME, Dept. ChiBioFarAm, in collaboration with the centre CASPE and associated Institutions. It will be the physical place to operate the prototype unit and use it as a showcase to demonstrate the technology. It will be led by the PI or a person designed by her. Initially, it will use the project resources to start the activities, which are planned to continue beyond the end of the project. One of the aims of the hub is thus also to find external resources to continue the activities.

3b. Showcase the project results

The main objective of the hub is to showcase the project technology with the aim of both **a**) presenting the results of the project and promoting it at various levels and **b**) demonstrating to both companies interested in investing in the technology to other Institutions which may collaborate for presenting projects together for further increasing TRL, and to public authorities and/or society the possibilities offered by the technology to accelerate the transformation to a carbon-neutral future.

3c. Dissemination and Communication

Although these activities are not limited to only experimental development, they are an integral part of the objectives of showcasing the technology, giving it visibility and rising interest.

3d. Assess exploitability and identification of an Exploitation Plan beyond the project

This activity aims to guide the developed solutions from a market perspective, identifying the requirements and constraints deriving from the different possible applications at an early stage. This activity first identifies and characterises key markets for each use case (continuous or on-demand production of H_2) by examining the commodities and services to be generated and marketed in each use case, starting from the desk study and in-depth project plan analysis. For each market, the main trends and conditions are then screened and described to understand their potential impact on the envisaged result of the use cases in the project. A PESTE (Political, Economic, Social, Technological, Legal and Environmental factors) framework identifies and characterises key factors and trends. In terms of SWOT analysis, the societal acceptability of the technology will be assessed with indications of aspects to remark on in dissemination activities.

3e. Business cases & exploitation strategy.

This activity aims to define the project results from a business case perspective by defining an exploitation strategy. It will also use approaches such as the Innovation Radar to define the exploitable items beyond the technology itself. The general activities include **i**) analysis of the current market connected with technology and identified application cases, **ii**) the definition of the initial project exploitation strategy, **iii**) the identification of project tangible and intangible results, **iv**) the definition of target markets and the suitable means for the project output to reach the market. In creating a preliminary business innovation plan for the project outcomes, the project will initially identify the value proposition of the results for the various (existing and emerging) market actors and evaluate those more suitable to commercialise the project results.

3f. Manage innovation and IPR within the project

Although a single partner is present (the Host Institution), aspects related to intellectual property rights (IPR) may still exist, including if an agreement with companies or other Institutions will be made to exploit the project results. For this reason, a series of activities towards defining a plan for the exploitation of the project's tangible and intangible results, as well as defining application cases and IPR, is part of the SCOOP plan of activities.

3g. Creating an Advisory Industrial Board for the project

In order to increase the effectiveness of the 3a-3f actions, it is planned to create a high-level **Advisory Industrial Board (AIB),** which will help the project better orient the project results along industrial needs early identifying the possible stakeholders and market opportunities, assist in raising the industrial interest in the project results. The initial composition for the AIB, which is planned to meet at least one time per year, is the following:

- Dina Lanzi, Head of Technical Business Unit Hydrogen of SNAM and vice-President of H2IT (Italian Association of Hydrogen), Italy
- Luigi Crema, Director of Centre Sustainable Energy of FBK, and President Hydrogen Europe Research, Italy
- Andrea Bombardi, Executive Vice President at RINA and board member of H2IT, Italy
- Mario Marchionna, Corporate Head of Technology Innovation di SAIPEM, Italy
- Sara Scagliotti, Head of Natural Resources, Wind and Marine Energy Res. Center, ENI, Italy
- Gerardi Cosimo, CTO 3SUN Gigafactory (Enel Green Power), Italy
- Giuseppe Monteforte, CTO A2A Energie Future, Italy
- Maximilian Fleischer, Chief Key Expert at Siemens Energy (Germany)
- Jan Mertens, Chief Science Officer at ENGIE (Belgium)

It is planned that about 30 PMs (person-months) among structured and project-hired researchers will be necessary to perform these activities in addition to external consultants.

Description of the workplan concerning the increase of the TRL

The Pert chart (Figure 6) and the above discussion already introduced the project structure, the planned activities and how they contribute to the expected increase of TRL from the starting value of 3 to a level of TRL in-between 5 and 6, e.g. prototype validation under environmentally relevant conditions. This plan of activities is translated into the workplan presented in Figure 9. The workplan is structured in three workpackages (WPs) corresponding to the three blocks of activities: WP1 (fundamental research), WP2 (industrial research up to prototype) and WP3 (experimental development). Each WP is structured in tasks corresponding to the actions described before.

The Gantt chart shown in Figure 12 reports the timing of each of these WP and task, the expected increase in the TRL during the task, and the person-months (PMs) requested for the task, divided between the UniME employees (E) and personnel hired (H) for the project.

Table 1 shows the breakdown of PMs for the various WPs and the type of personnel (full professor - PO, associate professor - PA and researcher for UniME employees, and post-doc and PhD for the hired personnel). A total of 190 PMs will be necessary to realise the planned activities.

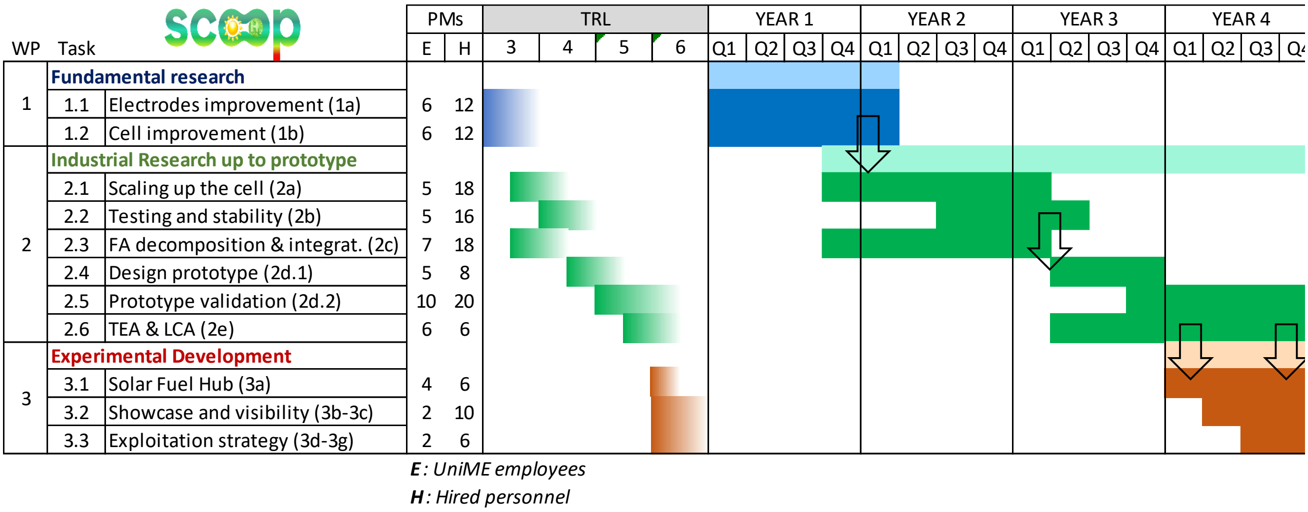


Figure 12 Gantt chart of the SCOOP project, with an indication of structure in workpackages (WPs), their timing and contribution to increasing the TRL, and the person-months (PMs) necessary to realise the activities.

Table 1 Breakdown of PMs for the various WPs and the type of personnel (full professor - PO, associate professor - PA and researcher for UniME employees, and post-doc and PhD for the hired personnel).

	WPs			
	1	2	3	
UniME employees				TOT
PO	6	9	3	18
PA	6	25	5	36
Res.	0	4	0	4
Hired personnel				
post-doc	12	36	12	60
PhD	12	50	10	72
TOT	36	124	30	**190**

The detailed person-months (PMs) and cost breakdown are reported in Table 2.

The description of the activities has been detailed before. Below is a detailed description of the main roles of the different personnel involved in the project (/w - women, /m - man):

UniME employees

- **PO** (S. Perathoner/w - principal investigator (PI); G. Centi/m, G. D'Angelo/w, R. Salomone/w; associated PIs): coordination of the activities, supervision and planning of the research, conception and design of the experiments, dissemination and communication, exploitation planning, supervision of reports and research costs, maintaining relations with AIB
- **PA** (P. Lanzafame/w, R. Passalacqua/w, S. Abate/m, C. Ampelli/m; Research Directors): day-to-day follow of PD and PhD, analysis and interpretation of the data, quality check, training younger researchers in equipment and testing, performing higher level tests, the definition of protocol for research and data collection, assist PIs in writing the research articles related to the project, and report directly to the PIs.

- **Res** (G. Papanikolau/w, C. Genovese/w, F. Tavella/m; Research Assistant): perform specific characterization tests and simulations for studying the electrocatalysts, electrodes and cell design

Hired personnel

- **Postdoc** (PD): planned to hire (in the four years of the project) 2-4 PD (or a hired RTT) for a total of 60 PMs. They will work under the direct supervision of PIs in collaboration with PA and Res. They will follow directly one or more PhD in their experimental work. They will also directly perform research for the planned activities.
- **PhD:** planned to fund with the project two PhD positions (36 PMs each) as part of the Industrial Doctorate ACCESS (UniME), starting from the 40 cycle. They will work under the direct supervision of a post-doc or a PA and report periodically to PIs that will supervise the overall research execution.

Table 2 Detailed breakdown of PMs and costs for the various WPs and activities by type of personnel (full professor - PO, associate professor - PA and researcher for UniME employees, and post-doc - PD - and PhD for the hired personnel).

		scoop	PMs - UniME pers.				PMs - Hired			Months		Cost € - UniME pers.				Cost € - Hired		
WP	Task		PO	PA	Res	TOT	PD	PhD	TOT	Start	End	PO	PA	Res	TOT	PD	PhD	TOT
	Fundamental research																	
1	1.1	Electrodes improvement (1a)	3	3		6	6	6	12	M1	M15	32.448 €	18.688 €	0 €	51.136 €	27.000 €	12.500 €	39.500 €
	1.2	Cell improvement (1b)	3	3		6	6	6	12	M1	M15	32.448 €	18.688 €	0 €	51.136 €	27.000 €	12.500 €	39.500 €
	Industrial Research up to prototype																	
	2.1	Scaling up the cell (2a)	2	4		6	10	8	18	M9	M27	21.632 €	24.918 €	0 €	46.550 €	45.000 €	16.667 €	61.667 €
	2.2	Testing and stability (2b)	1	3		4	7	10	17	M19	M30	10.816 €	18.688 €	0 €	29.504 €	31.500 €	20.833 €	52.333 €
2	2.3	FA decomposition & integrat. (2c)	1	4	2	7	4	8	12	M9	M27	10.816 €	24.918 €	8.648 €	44.381 €	18.000 €	16.667 €	34.667 €
	2.4	Design prototype (2d.1)	2	5		7	4	5	9	M27	M36	21.632 €	31.147 €	0 €	52.779 €	18.000 €	10.417 €	28.417 €
	2.5	Prototype validation (2d.2)	2	5	2	9	7	14	21	M33	M48	21.632 €	31.147 €	8.648 €	61.427 €	31.500 €	29.167 €	60.667 €
	2.6	TEA & LCA (2e)	1	4		5	4	5	9	M27	M48	10.816 €	24.918 €	0 €	35.734 €	18.000 €	10.417 €	28.417 €
	Experimental Development																	
	3.1	Solar Fuel Hub (3a)	1	2		3	2	4	6	M37	M48	10.816 €	12.459 €	0 €	23.275 €	9.000 €	8.333 €	17.333 €
3	3.2	Showcase and visibility (3b-3c)	1	2		3	6	4	10	M40	M48	10.816 €	12.459 €	0 €	23.275 €	27.000 €	8.333 €	35.333 €
	3.3	Exploitation strategy (3d-3g)	1	1		2	4	2	6	M42	M48	10.816 €	6.229 €	0 €	17.045 €	18.000 €	4.167 €	22.167 €
		TOT Fundamental research	6	6		12	12	12	24			64.896 €	37.377 €	0 €	102.272 €	54.000 €	25.000 €	79.000 €
		TOT Industrial Research	9	25	4	38	36	50	86			97.343 €	155.735 €	17.295 €	270.374 €	162.000 €	104.167 €	266.167 €
		TOT Experimental Development	3	5		8	12	10	22			32.448 €	31.147 €	0 €	63.595 €	54.000 €	20.833 €	74.833 €
		TOT	18	36	4	58	60	72	132			194.687 €	224.259 €	17.295 €	436.241 €	270.000 €	150.000 €	420.000 €

Estimated costs concerning the planned activities

Based on the PMs breakdown indicated in Table 1, the actual cost for the UniME employees involved in the project (of the CASPE laboratory) and for the personnel to hire is shown in Table 2 and summarized in Table 3. Note that these costs refer to present costs that may slightly change in the future depending on salary adjustments and some minor modifications in the personnel involved in the specific activities.

The POs involved in the project are four (S. Perathoner, G. Centi, R. Salomone, G. D'Angelo), four the PAs (S. Abate, P. Lanzafame, R. Passalacqua, C. Ampelli), three the researchers (G. Papanikolaou, C. Genovese, F. Tavella). Post-doc PMs correspond to 5 annuities (5x12) and those of PhD to 2 positions (2x36). The UniME employees are of the SSD (scientific disciplinary sector) CHIM/04 (Industrial Chemistry), ING-IND/25 (chemical engineering), FIS/01 (experimental physics, G. D'Angelo), and SECS-P/13 (economy, R. Salomone).

For equipment, amortisation is reported considering 45 months on 60 (5 years), 100% use in the project. For WP1, a gas-chromatograph (full cost 55 k€) would be necessary for the testing apparatus. For WP2, the control and analytical systems for the FA decomposition unit, solar simulator and electronic control systems for the cell (full cost 79 k€ in total) are necessary.

Consultancy costs (35 k€) refer to those indicated above for an expert in techno-economic assessment and design of the prototype unit.

Other operating costs refer to:

(i) WP1 - 5 k€ for consumables (chemicals, gas, spare parts laboratory) necessary for the preparation and testing of the electrodes and cell, 3 k€ related to mobility and dissemination for the project, 2,2 k€ for open science costs.

(ii) WP2 - 35 k€ for consumables (chemicals, gas, spare parts laboratory) necessary for prototype operations, 453,8 k€ for procurement of the PV module and manufacture of the prototype, 7 k€ related to mobility and dissemination for the project, 6 k€ for open science costs.

(iii) WP3 - 8 k€ for communication and dissemination activities of the *Solar fuel hub* (website, communication material, etc.) and managing showcase activities, 5,4 k€ related to mobility and dissemination for the project.

As the call indicates, overheads are calculated at a 25% flat rate.

Table 3 Cost breakdown for the various WPs based on the cost categories indicated in the call. See the text for the explanations.

Costs, €

	Personnel		Equipment	Consult.	Others	Overh.	TOT
WPs	Employeers	Hired	Ammort.		Mater., etc.		
1	102.272 €	79.000 €	41.175 €	0 €	10.152 €	58.150 €	290.749 €
2	270.374 €	266.167 €	59.475 €	35.000 €	501.799 €	283.204 €	1.416.019 €
3	63.595 €	74.833 €	0 €	0 €	13.421 €	37.962 €	189.811 €
TOT	436.241 €	420.000 €	100.650 €	35.000 €	525.372 €	379.316 €	1.896.579 €

The total estimated costs are about 1.90 M€, of which 75% are for WP2 (Industrial Research), 15% are for WP1 (Fundamental Research), and 10% are for WP3 (Experimental Development).

The breakdown of the *costs for the procurement of the prototype* is reported below and Table 4:

- Procurement (subcontract to Jülich) of PV modules for use in the lab-scale and prototype unit: 41 k€
- For prototype manufacture (subcontract to Hysitech): see details in Table 4

Table 4 Cost breakdown for manufacturing and procuring the prototype unit to validate the SCOOP project results (costs are in k€).

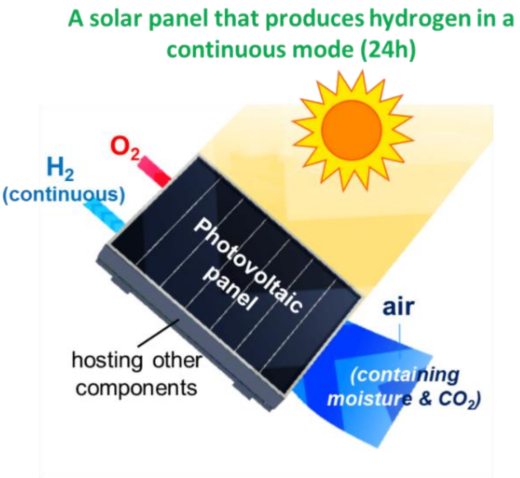
	k€
PV modules (lab-scale cell and prototype unit)	41,0
Tubes-pipes-fittings	12,0
Structural steel, Metal sheets for vessels	25,0
Raw Plastic Materials	10,0
Wires, Cables, Insulation	15,0
Sensors, Valves, Safety elements	34,0
Pumps and Vessels	35,0
Control devices, Electrical Components, Software of control	52,8
Housing and assembling	43,0
P&ID, design	25,0
Safety analysis and preliminary testing	25,0
Electronic for control and remote monitoring	38,0
Analytical on-line equipments for continuous monitoring	88,0
Consumables for initial tests	6,0
Transport and delivery	4,0
TOT	**453,8**

Beyond the project, the path to commercialisation

The project results will demonstrate the feasibility at TRL 5-6, with an estimation of the costs and environmental benefits of the proposed technology. The path to commercialisation will require further study to realise a commercial-sized unit. However, it will likely require realising a spin-off company or agreement with existing companies interested in exploiting the technology. Various EU calls are also suited for such a further increase in TRL. The path to commercialization will rely on the input and indications of the *Advisory Industrial Board* (AIB), see pag. 26.

It is useful to indicate the possible final solutions that can be foreseen for the device. For the prototype testing, the various components of the technology are separate elements (Fig. 11) to allow better modification and optimization, the commercial unit should integrate all of them into a single unit. The idea is to have PV panels which integrate on the back side of the other necessary components to allow the continuous production of H_2 without having the necessity of other connections, and thus the possibility to be installed, for example, on the roof of the buildings. This is presented schematically in Figure 13. To avoid having connections to the water supply, it is also possible to consider that the water molecules in the air are captured (particularly during the night) by the panel when the airstream enters the device. This technology is already being developed for other uses (for example, to capture water from the air in the desert).

While some spin-offs are trying to develop systems which integrate a PV module with an electrolysis unit to produce H_2 (for example, Solhyd spin-off in Belgium, and recently KTI in Germany), their limit is the production of hydrogen only during the day, while almost all applications, from building to industry, agriculture, energy communities, etc. will need to have hydrogen especially during the night or in a continuous way. The solution developed within the SCOOP project may thus also be an upgrade of the solutions developed by these companies. The PI and her team are known well the founder of Solhyd (prof. J. Martens); thus, possible collaborations in this direction are highly facilitated. These solar panels are estimated to produce about 250 litres of hydrogen daily. With the actual decrease in the costs of PV modules and the fact that other necessary components are expected to increase by about 30-40% of the total cost, the solution proposed is expected to be competitive for applications such as building, energy communities and agriculture.



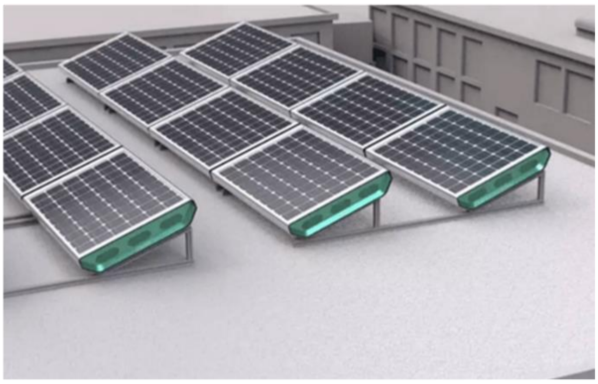


Figure 13 Conceptual rendering of the possible commercial development of solar panels producing hydrogen continuously (elaborated from Solhyd).

The storage of H_2 as FA also allows the *production of H_2 may be modulated on demand* rather than produce H_2 in a continuous mode. This great flexibility of operations overcoming the limits of the PV + electrolyser solution, which needs intermediate storage of H_2 to allow the same flexibility of operations, is the main advantage from a commercial perspective of the solution proposed within the SCOOP project.

SECTION 3

State-of-the-art

Artificial photosynthesis to convert carbon dioxide (CO_2) and water directly into value-added chemicals is one of today's dream challenges to meet growing energy demands and curb climate change due to the accumulation of CO_2 in the environment.[14-16] In general, "artificial leaves" (ALs) are small-scale reactors involving the electrocatalytic transformation of abundant small molecules (i.e., water, carbon dioxide, dinitrogen, and methane) by using renewable sources such as solar power.[17] Although often claimed that they should mimic the natural photosynthesis process, it is necessary to intensify the process efficiency and rate largely by at least one order of magnitude to realise a device that can be cost-effective.[18] For the same motivation and to develop sustainable ALs, it is critical to use earth-abundant materials for the construction of these devices and electrodes [COM(2020) 474 - Critical Raw Materials Resilience, European Commission, 2020] as well as the adoption of cell engineering and design suitable for easy scale-up and mass production, also avoiding the use of sacrificial donors or electrical bias.[19] Stability is another important requirement, which implies using stable materials, cell design, and operating conditions to enable long-term operations.

Hydrogen (H_2) is considered the simplest fuel generated from an AL. Khaselev and Turner already studied direct water electrolysis in 1998. They reported an integrated-monolithic photoelectrochemical-photovoltaic device with 12.4 % hydrogen efficiency at 11 suns of light irradiation using rare earth elements to prepare the electrodes (i.e., $GaInP_2$/GaAs).[20] However, the pioneering device for artificial photosynthesis was the cell introduced by Nocera's group over ten years later, unveiling the first practical artificial leaf (working at one sun in near-neutral pH conditions) for water splitting with 5 % solar efficiency.[21] This cell was made of cheap materials but focused on only hydrogen production and stability issues related to photo corrosion of the integrated PV cell immersed in the electrolyte.

Several studies have been made later, and an overview of the different results is presented in Figure 14.[22] This Figure summarises the results of η_{STH} (efficiency in solar to hydrogen - STG as a function of the arbitrary index of system complexity, allowing for clustering together results as a function of the system architecture (PP, PEC, PV/EC, e.g. the use of the catalyst in the particulate form, suspended in water - PP, photoelectrochemical configurations - PEC and combination of a photovoltaic unit and an electrochemical cell - PV/EC). The indicative region (in green) representing potential interest from a practical perspective is also outlined. This Figure provides a quick view of the state-of-the-art and the performances as a function of the device architecture. Details are given in ref.[22], indicating the type of materials used, current densities and other relevant aspects.

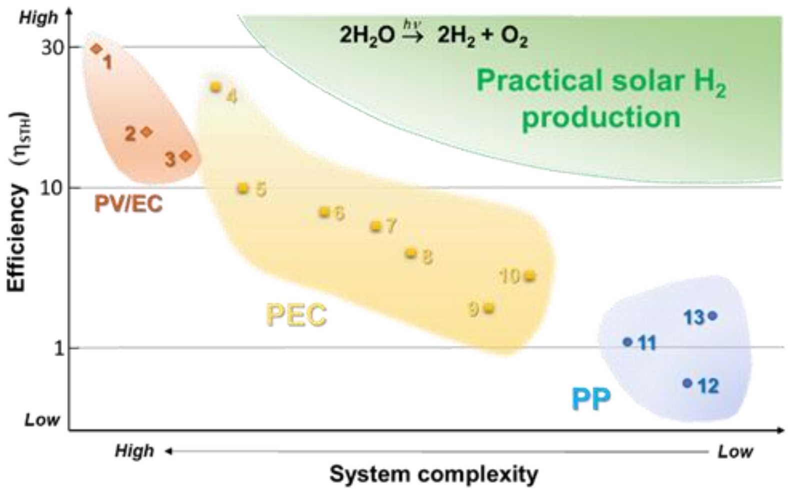


Figure 14. Summary of representative results about H2 production through PP, PEC and PV/EC approaches. See ref.[22] for details

The highest performances come from PV/EC systems, where η_{STH} ~ 30% has been demonstrated by using a commercially available InGaP/GaAs/GaInNAs(Sb) triple-junction solar cell, at 42 SUNs (delivering a JSC = 584 mA·cm^{-2}), connected in series to two polymer electrolyte membrane (PEM) electrolysers.[23] Although such performances represent a remarkable result, the authors report a JSC of ~14 mA·cm^{-2} at 1 SUN, which is significantly lower than the theoretical limit of the photocurrent for this kind of PV unit.

Another recent work highlighted the high potential of the PV/EC architecture in water splitting by exploiting an InGaP/InGaAs/Ge solar cell and an electrolyte-less EC based on an $IrRuO_x$-Pt catalyst.[24] The authors reported a JSC of 5.49 A·cm^{-2} (at 474 SUNs), an impressive Jop of 0.88 A·cm^{-2} and a η_{STH} = 17.12%. The about 500 times solar concentration requires proper thermal management of the system. Indeed, the authors report JSC = 13.9 mA·cm$^{-2,}$ which is lower than the expected limit of this kind of multi-junction solar cell.

These considerations should be integrated with the analysis of J (current density) to derive reliable conclusions on the more promising materials and approaches. The indication emerging from this combined analysis[22] is that for the water splitting case, the PV/EC architecture allows obtaining high-J and η_{STH}, especially when coupled to a concentrator system and a proper heat management system, which largely increases the costs. Furthermore, performance losses after long-lasting use must be accurately assessed (such as the detachment of catalyst particles and membrane degradation).[23] For these reasons, even if high η_{STH} and apparently very promising data have been reported in the literature, none have reached commercial or pilot-scale experimentation.

Still, the simple combination of commercial PV modules and electrolysers is the preferable solution, even if coupling may not be optimal. On this approach, research on a small-scale pilot scale, such as the cited Solhyd SME and other small innovative companies (SunHydrogen, SunGreenH_2, Heliogen/Bloom Energy, etc.)[25] focus recently. This solution appears preferable regarding the cost of production of the green H_2 and lower environmental impact.[25]

However, these solutions do not address the problem of H_2 storage and discontinuity in producing H_2. Still, it is the main factor limiting the market perspectives.

A modified PV-EC approach allows converting CO_2 to formic acid (FA).[22] FA allows a high volumetric H_2 storage capacity of 53 g_{H2} L^{-1}, and relatively low toxicity and flammability for low-cost and convenient hydrogen storage and transportation.[26-28] From this perspective, the combined production of formate and H_2 in an efficient AL-type device is an attractive solution because it can produce both green H_2 and a hydrogen carrier that is easy to store. Such a device can be integrated into distributed networks of green H_2, with the fluctuations in H_2 production due to sunlight variability mitigated by using the hydrogen carrier. CO_2 can then be closed-up by recirculating it.

This solution presents advantages over the combinations of PV or wind, electrical energy storage and water electrolysers to produce H_2 continuously or on demand. However, it is a largely unexplored option, and there is still a lack of devices with suitable characteristics for this technology. In this sense, the combined and balanced production of formate and H_2 with high solar-to-fuel efficiency is the target, rather than the Faradaic Efficiency (FE) to formate. However, the C-selectivity to formate, i.e., the selectivity of converting CO_2 to formate rather than other C-products such as CO, methanol and higher alcohols, hydrocarbons, etc., is required.

One of the most recent PEC approaches for selective formate generation was developed by Domen's group, reporting a scalable CO_2 reduction process using a molecular-based hybrid photocatalyst with a remarkable selectivity to formate (97 ± 3 %).[28] However, critical raw materials were used to prepare the electrodes (i.e., $SrTiO_3$:La, Rh) and a very low solar-to-formate efficiency was obtained (0.08 ± 0.01%). In 2016, Zhou et al. reported a 10 % energy-conversion efficiency with a current density of about 9 mA·cm^{-2} but using costly InGaP/GaAs PV component, a noble metal-based cathode and very small electrode surface area (0.03 cm^2), i.e. not amenable to large-scale application.[29] Furthermore, Piao et al. reported an overall solar conversion efficiency of about 8.5 % with a current density of about 10 mA·cm^{-2} but using expensive electrodes (i.e., IrO_2 as the anode) and chlorite-promoted electrolyte (with corrosion and safety issues for the possible formation of Cl_2).[30] Recently, Kato et al.[31] reported a solar-driven electrochemical reduction of CO_2 to formate with a conversion efficiency of 7.2% using a Si-based PV cell, then scaled up to 1 m^2 eight-stacked electrodes with improved efficiency of 10.5%,[32] but also, in this case, costly noble-metal based electrodes (anodes based on IrO_x and cathodes on molecular Ru-complex polymer) were used. Examples of efficient artificial-leaf-type devices free of noble metals or expensive materials have not been reported for relatively high current density formate production. The balanced coproduction of formate and H_2 was also not investigated.

Originality and innovative character

This project aims to realize a novel solar-to-hydrogen conversion system that integrates hydrogen storage in formic acid to allow continuous (24h) hydrogen production or production on demand. From this perspective, it is a unique proposal because there is no equivalent undergoing study or literature data. They have limited their approach to coupling an H_2 electrolyzer with a PV module, thus making operations possible only when sunlight is present. On the other hand, there is no possibility of effective alternative H_2 storage (adding an external H_2 storage unit to the combination of a PV module and an H_2 electrolyzer), which allows for the realisation of an equivalent solution for small-scale integrated applications, as outlined in Figure 13.

The proposal derives from the results of a previous EU FET project (A-LEAF), which was focused on developing at TRL 3 a lab-scale bias-free PV/EC flow-cell for converting CO_2 and water into formic acid (FA) and O_2 under sunlight irradiation, using only earth-abundant materials. PV/EC architecture indicates a photovoltaic (PV) module integrated within the electrochemical cell but not in contact with the electrolyte to enable high stability of the PV component. In PEC (photo-electro-catalytic) cells, the PV unit directly interacts with the electrolyte or a semiconductor photoelectrode is directly used. A survey of state-of-the-art results indicates that PV/EC architecture is currently preferable.[22]

The PV/EC cell developed within the cited A-LEAF project works as an AL-type device at room temperature and atmospheric pressure. It has a highly compact design and is amenable to scale-up. It is integrated with gas diffusion electrodes based on Cu-S for CO_2 reduction and Ni-Fe-Zn oxide for water oxidation. The electrochemical part (EC) was successfully coupled with a low-cost PV four-cell module based on silicon heterojunction (SHJ) technology, leading to a full lab-scale prototype that delivers outstanding performance by converting over 6% sunlight into FA and an overall 10% solar-to-fuel efficiency also considering hydrogen production. FA is accumulated in the liquid phase at the EC part and separated from the gas outlet rich in H_2. The combined PV/EC device is the result of an optimized design and electrodes to (i) operate close to the maximum power point of the PV device, (ii) reach a cell voltage in the EC device high enough to drive the reduction/oxidation reactions, (iii) minimise energy losses due to overpotential, and (iv) control potentials within the stability limits of the catalysts.

SCOOP starts from these already innovative results, extending and validating them at higher TRL (5-6, Figure 12), but especially introducing a fully original concept of using the co-production of H_2 and FA as a way to integrate storage of H_2 for dark operations when H_2 can be produced by FA decomposition (Figure 1). There is no literature data or announced research activities by spin-offs or other companies for such a solution. As mentioned above, it can represent an important extension of current solar-to-hydrogen proposals. Thus, the implementation of the project results can be quickly realized when feasibility is demonstrated at a sufficient TRL level.

The innovative aspects of the proposal lie thus in (**i**) the cell and related materials for the combined production of H_2 and FA, and (**ii**) the integration of the cell is a process scheme allowing to store part of the H_2 as FA during sun illumination periods and produce then H_2 from FA during dark periods. All the components are already designed to realize a compact device as conceptually rendered in Figure 13, even if the realization of this integration is an aspect going beyond the SCOOP project.

Impact of the research activities

General impact and social relevance

Developing an energy and chemistry scenario beyond fossil fuels (FF) is emerging as a relevant industrial and social direction indicated by the EU to meet the Net-Zero-Emissions (NZE) target by the year 2050.[33] This target requires a full system transition, impacting the scientific perspective. In addition to new processes and materials, a framework of novel concepts, solutions and technologies is necessary. Among them, new solutions for producing green H_2 in a distributed way at competitive costs and overcoming the current limitations in the transport and storage of hydrogen is a global challenge to accelerate the transition to the new sustainable, carbon-neutral future. Current activities on green hydrogen focus on electrolysis along the possible implementation routes. While hydrogen vectors to store and transport are under development, they are a secondary process after the electrolysis step and represent an additional cost. Thus, combining cost reduction and limitations in using H_2 would require a different, innovative approach. Accelerate the introduction of green H_2 and the related social benefits, thus passing through the capability of developing innovative solutions overcoming the above limitations. *This is the aim of the SCOOP project and its social relevance*.

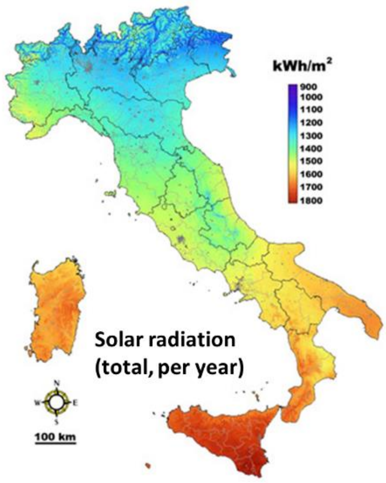
Making available effective solar-to-hydrogen (STH) solutions, which overcome the current limits in storage H_2, and make possible a continuous or on-demand production of hydrogen, makes it possible to develop many novel solutions for the vast and novel area of prosumers, e.g. producers and consumers of energy such as the energy communities. There are many applications with significant social relevance which may be indicated:

- *Buildings and energy communities*. Buildings require heating, cooling and electricity. These can be provided by hydrogen via combined heat and power (e.g. fuel cells) or a hydrogen boiler. Next to classical photovoltaics, hydrogen panels could be installed on roofs. The solar hydrogen is stored directly in the STH module, differently from solutions under development based on PV + electrolyzers, which demand the storage of external solutions of difficult use for distributed productions, as commented before. Compared to alternative technologies to utilize green hydrogen for the built environment, from fuel cells and hydrogen panels to heat pumps, batteries and hydrogen boilers, the proposed solution shows many potential advantages (as indicated in the final report of the BatHyBuild project, WaterstofNet - April 2021). Some of the key messages from this study, which remark the social impact of developing the SCOOP technology, are the following: (**i**) hydrogen is a valid choice for heating of buildings, and cost-competitive to electrical-only solutions, when storage of H_2 is solved as proposed by the SCOOP technology, (**ii**) hydrogen boilers consume no electricity for heating, thus lowering the electricity demand especially in winter, with benefits in realizing more stable and resilient energy grids, (**iii**) solar hydrogen enables to enhance the use of decentralized renewable energy production, because enhances the capacity of the electrical infrastructure to integrate solar energy overcoming current limitations, (**iv**) hydrogen-based heating solutions can often be competitive, when the issue of dependence on solar illumination is overcome, (**v**) hydrogen production overcoming the limits associated to hydrogen pipeline infrastructure becomes an important driver to accelerate the introduction of an hydrogen-economy, with the related social benefits. For local production of renewable hydrogen, the cited study indicates that from 20 to 50% of energy auto-consumption derives from guarantee continuity in supplying energy when H_2 is produced by electrolysis, while this energy demand could be virtually zero in the process solution proposed by the SCOOP project, thus enhancing overall energy efficiency in applications to buildings. For energy communities, local energy production is now mainstream. Islands, remote villages, and energy cooperatives are all examples of communities that could use hydrogen (panels) for local renewable energy production.
- *Mobility*. The distribution of hydrogen is the main limiting factor which has hindered the introduction of hydrogen-based solutions for mobility, which extend beyond only cars. The SCOOP solution, tailored for distributed continuous or on-demand production of H_2, can boost this solution.
- *Agriculture*. Nearly half of the available land surface area is occupied by agriculture. This space is required because plants need sunlight to grow. Luckily, enough sunlight is available to produce crops and energy on the same land via the agrivoltaics principle. As such, rural areas may provide food and renewable hydrogen.

- *Industry*. Decarbonization of many small-size productions cannot be realized with the current solutions. Novel approaches will be required to produce green H_2 in a distributed mode, with integrated hydrogen storage as proposed by the SCOOP project.
- *Off-grid*. Globally, over 1 billion people lack access to clean energy. Moreover, diesel fuel is imported to produce electricity in (backup) power generators in many locations, such as islands. Hydrogen panels would be able to provide on-site renewable hydrogen for various applications.

The technology proposed by the SCOOP project will thus, from one side, accelerate the introduction of a larger use of hydrogen in many applications by overcoming dependence on the grid and related large investments and, from the other side, introduce new solutions for decentralized energy management, in energy communities, offering additional possibilities which overcome the limits of only using renewable electrical energy.

The SCOOP technology is thus an enabler solution to introduce new solutions with high impact on society in terms of (**i**) reducing the carbon footprint, (**ii**) promoting employment and integration of energy production within the territory, (**iii**) resilience and cost mitigation by avoiding the dependence from an external supplier and the existence of a grid.

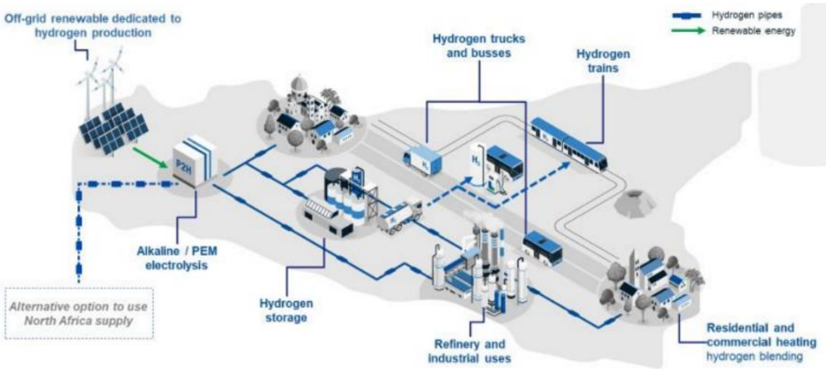


SCOOP thus contributes significantly to resolving important social problems and accelerates the transition to a carbon-neutral future.

The relevance for Sicily

Sicily has a natural vocation to renewable energy from the sun. As shown nearby, the solar radiation in Sicily is nearly two times higher than the average in Italy. There are also large areas in the inner part of Italy where solar fields can be created. At the same time, the production of renewable electrical energy is hindered by transport to regions (in the north of Italy or Europe) where this potential can be exploited. *Thus, this large potential remains largely unexploited due to the limitations in transporting and storing renewable energy.*

Overcoming this limitation could have thus a large and significant impact on a *recovery plan* to convert the current energy production in Sicily, largely based on fossil fuels (various refineries and energy plants are currently in severe crisis impacting directly over 5,000 jobs plus the induct). Revitalizing this area through the shift to hydrogen production in a transportable form becomes the enabling element of the transformation that combines knowledge resources with the needs of society and industry.



SNAM has chosen Sicily as the reference case for creating a hydrogen hub (The potential of hydrogen in Italy; Snam and McKinsey, Oct. 2019). Although they do not consider the possibility of the SCOOP technology, their analysis is further reinforced by the possibilities offered by the proposed solution. Among the benefits of creating this hydrogen hub in Sicily are (**i**) a reduction of 1,250 k tons of CO_2 per year, (**ii**) the boosting of the local value chain and jobs related to the development of the assets, operations and maintenance during asset lifecycle, attractiveness to international investments (e.g., ammonia producers) to open plants in Sicily, (**iii**) end users benefits, from cost-competitive energy to reduction of the environmental impact and greenhouse gas (GHG) emissions, (**iv**) balancing services, by leveraging curtail power from increasing solar and wind renewables production for cheaper hydrogen production during curtail hours. This will help to manage the supply-demand unbalancing period, (**v**) tourism attractiveness, helping Sicily's image perception as a "green island".

Although the SCOOP project will contribute partly to realizing this potential impact, it will be relevant in demonstrating (showcasing) the possibility of novel low-cost solutions that can find new investors outside the traditional market, as it happened for PV fields.

Impact on the strategies of sustainable development and resilience in Sicily

In Sicily, the fossil-based energy production and transport sectors are the most polluting ones (ARPA Sicilia, 2018), contributing to around 44% of the share of the CO_2 emissions by sector in Sicily. Therefore, energy production from RES (renewable energy sources) could play a major role in protecting the environment while producing wealth, creating jobs, reducing GHGs emissions and improving the local economy. The Zonal Price for the Sicily market area was around 13% higher than the PUN (Single National Price). This higher energy price, even if the total net electricity production in Sicily was 15.863,4 GWh/year (in 2018), 5.255,1 GWh/year from renewable sources, e.g., 33.1% of the total.

The Sicilian Region's PEARS (Environmental Energy Plan) indicates that almost 70% of regional energy needs should be derived from using RES in 2035. This ambitious target cannot be reached by only producing renewable electrical energy. Thus, this target requires developing a strategy for producing energy vectors that can overcome limitations in fluctuations of RES production. In Sicily, the capability to store large amounts of electrical energy is limited. Sicily required a total of 20000 GWh of electricity. As shown in Figure 15, during the year, the sum of the wind power and the photovoltaic power at any time is never greater than the power required by the load.

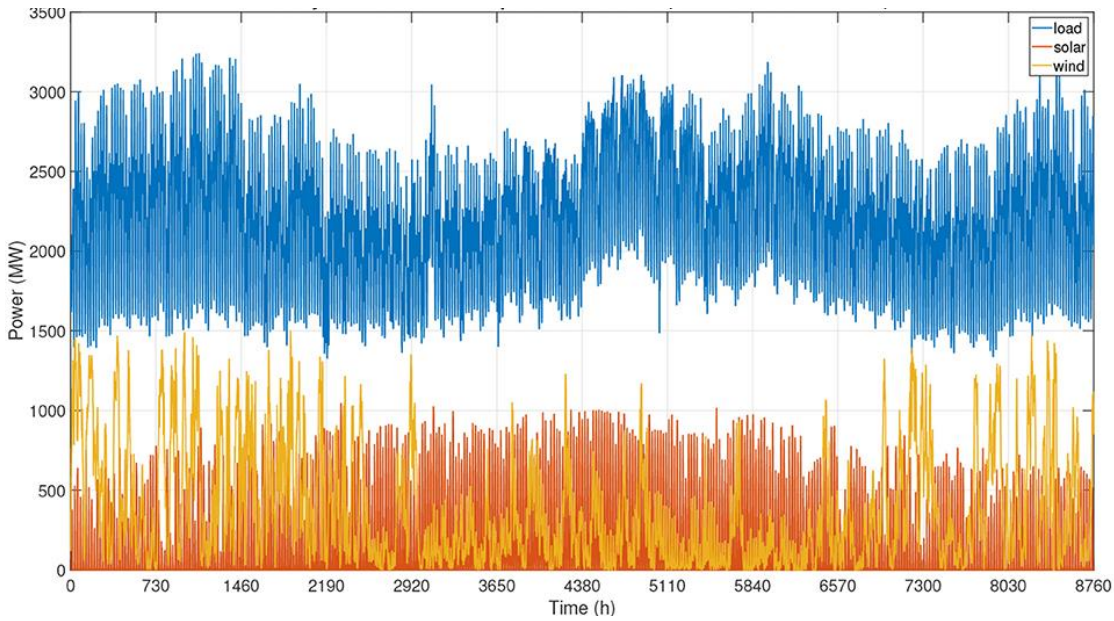


Figure 15. Sicily load and renewable production in 2018. Corrected ENTSO-E data from the Open Power System Data, 2020.

It may be estimated that the storage capacity should correspond to about 4-5 GW to compensate for the deficit, reach the target indicated by PEAR and stabilize the grid against fluctuations between load and production. It is largely unlikely that this target could be reached from the current electrical energy storage systems. Currently, there is only 170 GW of installed storage capacity worldwide, but more than 96% is provided by pumped hydro,[6] of which relevance for Sicily is minor. Other electrochemical, thermal and mechanical storage systems would require unrealistic high investments. Thus, pushing the introduction of energy vectors is crucial for a strategy of sustainable development and resilience in Sicily. Hydrogen would require, however, to overcome the limits of local storage, and need distribution through the pipeline to become an effective solution, even considering transport together with methane.

Thus, the SCOOP technology, overcoming these limits and favouring a distributed (low-cost) hydrogen production with intrinsic H_2 storage, represents thus a **strategic component** to enable Sicily to reach planned PEARS targets. These targets are crucial to **meet sustainability and resilience** from an energy perspective.

Impact on human capital and scientific excellence

This FISA proposal is led by PI S. Perathoner, director of the catalysis centre CASPE at the University of Messina (a joint centre between Univ. Messina, the Consortium INSTM and the European Research Institute of Catalysis). It will involve most of the researchers involved in CASPE, formed by about eight professors/researchers and about 15-20 PhD, post-docs and visiting researchers. The research group led by S. Perathoner as PI is among the pioneering groups developing electrocatalytic and Al-type devices for CO_2 conversion, as testified by the several publications and coordination or participation in several EU projects on these topics. These previous works constitute the solid knowledge background established by international collaborations on these topics. However, this project represents a step forward regarding specific development and applicative content. CASPE centre is thus among the *excellence centres* on the project topics. The PI and CASPE personnel are in first place in Sicily among the researchers, based on the Stanford University-Elsevier study (2022), on energy and hydrogen production. They were a member of the hydrogen working group of the Ministry of Research and University for the preparation of an Italian Hydrogen Research Strategy (SIRI) and a member of the Regional Observatory on Hydrogen of the Region Sicily, besides being involved in various activities and projects at EU or national level on hydrogen and devices for solar to fuel conversion.

The SCOOP project will thus further strengthen the excellence of this centre with an impact on the centre's scientific activities and human capital. In fact, over ten young researchers, between PhD and post-docs, will be hired on the project. They will work in a highly dynamic and internationally-oriented research team, thus significantly enhancing the human capital in a critical area for local development, such as green hydrogen, solar fuels and renewable energy.

Promoting human capital, particularly qualified human capital, is a crucial objective of the CASPE centre. As reported in the study by Svimez (2020), between 2002 and 2018, about 52,000 people accounted for the negative migratory balance for Sicily. Approximately 11,000 are graduates, with a dramatic economic and social cost. The employment gap between Sicily and Northern Italy has widened recently, especially the qualified one. The CASPE centre is therefore conceived as an engine for the development of the territory and human capital (with a direct impact in reducing the migration of students and graduates) to become the enabling structure for existing and future sectoral and territorial development plans, in the PNRR and European context.

The CASPE centre is anchored to the territory but has an international vocation and strong relational skills towards research and industry. Strengthening its capabilities on green hydrogen and solar-to-fuel conversion will enable technologies capable of being functional to promote innovation and minimization impact. This centre combines i) a demonstrated capacity for innovation in the strategic sectors of materials, technologies and devices for energy and the circular economy, engineering and evaluation of systems and processes, environmental and geological monitoring, etc., ii) an extensive existing network of collaboration at the national and international level, iii) a documented planning capacity at European level and with large industries, which, enhanced by the partnership, creates a new proactive model of innovation, acting as an incubator of ideas, projects and enabling technologies.

Credibility of the scientific impact

Artificial leaf (AL, or artificial photosynthesis) is a new technology for making fuels or chemicals from CO_2 and H_2O using direct solar energy. The SCOOP project uses the knowledge generated from an EU FET project that ended last year (A-LEAF) to build a new novel solution, developed up to TREL 5-6, to continuously produce (solar) H2 or on-demand. Besides offering a novel solution to produce solar H_2 and overcome the current limitations related to the intermittent nature of solar radiation, the project will contribute to the general field of AL-type devices and specifically to producing "solar" FA by converting

CO_2. AL technology plays a key role for:

1. *Clean energy sector*: coupled with FA fuel cells to transport renewable energy from remote areas or realize local storage of renewable energy to mitigate fluctuations.
2. *H_2 economy*: as hydrogen vector: to enable its remote production and the transport/storage, thus for H_2 uses which cannot be directly connected to a hydrogen grid.
3. *Circular economy*: by closing the C cycle in energy-intensive industries: cement, steel, refinery, chemical process sectors) by reusing the emitted CO_2 to convert to products used internally or in industries in symbiosis.
4. *Carbon-neutral production*: to produce alternative (low-carbon) chemicals/additives.

These applications belong to not yet established (or even growing) markets since green FA production (from CO_2 and solar energy) does not exist at the industrial level. No competitive technologies on the market can be used for this purpose. Although ALs are considered a key technology for a sustainable future, most current studies are still far from the level required to make business cases, even if non-EU companies such as Toyota[31, 32] are investing considerably in the area. EIC has launched (awarding in 2022) a 5 M€ prize and context to build an AL-type prototype that can produce useable synthetic fuel. This area is considered crucial to **i**) stimulate innovation in energy technology, **ii**) promote public and commercial interest, **iii**) accelerate the development of new innovative energy conversion systems using solar light to produce renewable fuels, **iv**) push the AL technology for fuel production to the next level of development, **v**) generate interest in the subject and foster interdisciplinary collaboration, **vi**) highlight the diversity of potential solutions.

The SCOOP project will develop a prototype to demonstrate the feasibility of a frontrunning technology to produce in a continuous mode H_2, which can also be used as a high STF efficiency device to convert CO_2 to FA using direct solar energy.

While there is a potential business and market fit for the technology, the technology is the prerequisite to stimulate the creation of the market and enable business cases. AL topic acts as a "game-changer" rather than being a novel but incremental technology for which a business case can be made. The potential is large, with several companies actively working in the field (TRANSPARENCY Market report "Artificial Leaf Market - Global Industry Analysis" indicates key players in the global artificial leaf market Toshiba, Evonik Ind. AG, Air Liquide, among others), but this is a very dynamic situation. The estimated potential market is over B€.

SCOOP will be the first novel technology validated at this TRL level in an area with large business and market opportunities. The project will demonstrate the possibility of having compact and low-cost integrated devices for continuous (or on-demand) solar H_2 production. At the same time, the project will also generate knowledge and prototype results for a highly efficient STF technology based on using earth-abundant materials and exploiting a cell engineering and design suitable for industrialization. SCOOP has the full features to address future commercialisation.

Driving toward a solar fuel market

A multi-step strategy for market innovation in solar H_2, AL devices and solar fuels/chemicals solutions can be identified to

i) manufacture and operate a prototype (TRL 5-6) to demonstrate and showcase the feasibility of the technology for distributed green H_2 production;
ii) analyze specific subsectors among the main areas which can be identified to exploit the project results: **1.** devices for producing H_2 in a continuous or on-demand mode; **2.** materials and electrodes for solar-to-fuel conversion; **3.** AL-type devices for converting CO_2;
iii) evaluate the impact and opportunities of the technology concerning main gaps and opportunities in substituting fossil fuels as the backbone for society;
iv) develop progressively the technology, societal and industrial bases to create a new value chain based on green H_2, AL and solar fuels.

The SCOOP project focuses on the first aspect but aims for a larger impact, demonstrating feasibility that catalyses further activities. The *Solar Fuels Hub* will be central to guarantee these aspects beyond the project itself.

Socio-economic and/or industrial context of reference

Economic and/or societal benefits

The global solar energy market is projected to reach $223.3 billion by 2026, growing at a CAGR (Compound annual growth rate) of ~20% in the next five years. In a net-zero emission scenario by 2050, IEA estimated for the year 2030 a global installed solar PV capacity of about 4000 GW. However, the analysis of production versus geographical and temporal demand shows that such an expansion (required to reach the target 55 % reduction in the European Union's emissions by 2030) cannot be reached without a significant introduction of energy storage on an annual basis and long-distance transport, as offered by solar fuels. In addition, beyond 2035-2040, the costs for decarbonising hard-to-abate sectors will be quite high without developing innovative solutions to produce solar fuels (particularly solar H_2) overcoming the many current limits (McKinsey, Net-Zero Europe). Assuming ≥10% GHG reduction for the year 2050 deriving from solar fuels, they should contribute to ~70-100 Mtons of CO_2 eq. reduction concerning current levels of emissions.

AL introduces a potential economical solution deriving from process intensification and the direct use of sunlight. SCOOP adds further innovation of on-site storage, allowing continuous or on-demand production of H_2. The project will also boost the development of AL-type solutions. As in AL devices, single-step solar-driven conversion introduces a novel path to reduce CAPEX and OPEX. SCOOP will demonstrate at prototype level and significant scale the possibility of obtaining a high STF efficiency and productivity, validating it under different cases. The project will thus provide reliable estimations on the future role of AL in reaching EU targets.

In parallel, dissemination and communication to researchers, stakeholders, and society is another crucial element of the project to create a market (and business) for green H_2 and AL technology and its role in meeting EU targets on climate change mitigation. From the societal perspective, in addition to the contribution to CO_2 eq. reduction, the role of green H_2 and AL technology will contribute to promoting a distributed energy and chemistry system, clean energy districts (or valleys), and better use of local resources of the territory (including waste CO_2), all with a positive impact on employment and societal involvement in energy management (changing from consumers to prosumers). By accelerating the energy transitions by introducing AL technologies and solar fuels, an impact of >0.3 M jobs in 2040-45 may be estimated using the EU report "Employment in the Energy Sector".

Techno-economic feasibility and estimation of its impact are thus the prerequisites to implement this scenario. SCOOP will enable this new path rather than acting only as a marketable technology. SCOOP will contribute to new European markets and related positive impacts (employment, societal, environmental, scientific).

Investment readiness

The SCOOP project aims to mature a specific commercial technology (panels for solar-to-hydrogen with incorporated storage capability). However, for its novelty, this is not an already established market. For this reason, a parallel aim is to develop disruptive technology to boost and accelerate the green H2, AL and solar fuels area, which will play an important role in the future sustainable society: a game-changer.

According to the call, this is a single PI and partner application project. It will thus prepare the scientific and technological bases for the technology, developing it up to TRL 5-6. However, further development up to a commercial scale will require exploitation agreements with companies or, eventually, dedicated grants for increasing TRL.

Impact on the industrial context

Enel Green Power is transforming its current solar panel factory in Catania into a Gigafactory to become

Europe's largest factory producing high-performance bifacial photovoltaic modules. The factory's production capacity is set to increase 15-fold to 3 GW/year from the current 200 MW through an investment of around 600 million euros. The Gigafactory is expected to increase local employment by around 1,000 jobs, catalysing the European PV value chain. The project will foster next-generation high-efficiency solar technology in Europe and contribute to reducing the continent's energy dependency. The University of Messina has a framework agreement for collaboration with Enel Green Power.

The three GW of panels to be manufactured every year by the Gigafactory can generate up to approximately 5.5 TWh of renewable electricity per year, which, from a sustainability point of view, has the potential to avoid the equivalent of up to almost 25 million tons of CO_2 in their first ten years of operation. Likewise, the output generated by the Gigafactory's panels has the potential to avoid the purchase of up to almost 1.2 billion cubic meters of gas per year, replaced by domestically-produced renewable energy.

In front of this large potential, the direct impact on Sicily and Italy will be minor because over 90% of these panels are expected to be installed out of Italy, for the limitations existing on the capability to share a significantly larger fraction of PV electrical energy production without the development of adequate storage capacities.

The SCOOP project offers the possibility of integrating these PV modules within a relatively simple housing (outlined in Figure 10), enabling the production of H_2 instead of electrical energy and with an integrated storage capability that allows continuous (or on-demand) production of H_2. The estimated costs for converting solar-to--electricity to solar-to-hydrogen are below an additional cost of 30-50%, thus enabling a cost-competitive production of green H_2 (below 4-5 €/kg).

Therefore, the SCOOP project offers a potential new market to Enel Green Power, with benefits on its industrial leadership and impact on employment, while at the same time enabling an effective path to foster the use of these panels in Sicily and Italy, with the related environmental benefits, increase in energy resilience and reduction on the dependence on fossil fuels.

Protecting the results and dissemination/communication strategies

Strong care is given at UniME to intellectual property rights (IPR). Although these are single-partner projects, thus limiting issues on these aspects, the project has a defined strategy for intellectual property management, ownership of the results and rules for the protection or dissemination of the results. The overarching rule is to protect the University's interests in this sensitive area while simultaneously creating all the conditions for exploiting the results in agreement with potentially interested companies. A mix of solutions will be considered to protect confidential results, such as patents, design rights, copyrights, trade secrets, etc. These measures will be a prerequisite for the exploitation strategy. At the same time, we are well aware that public dissemination (to scientific and stakeholder communities and society) is a crucial aspect in this important area for the sustainable future of society. Thus, an active communication and dissemination strategy is part of the project.

By creating the Solar Fuel Hub, communication measures will promote the project throughout its full lifespan and beyond. The project will inform and reach out to society to disseminate the activities performed, highlighting the use and benefits of H_2 and AL for citizens. The project follows Open Science targets but accounts for IP rights and interests of companies possibly interested in using the project results, as the cited Enel Green Power. Activities will be strategically planned, with clear objectives, starting at the outset and continuing through the project's lifetime.

The dissemination plan will report the strategy to engage stakeholders in the scientific, technological and industrial environments. Beyond these targets, the project will also participate in outreach activities to help raise public and societal awareness of carbon-neutral technologies, sustainability, circular economy, green solar hydrogen AL and solar fuels. All these concepts are strong and relevant parts of our proposal. We will contribute to spreading good practices and positive uptake of the new technologies in this needed societal transformation. Various scientists involved in this project have already conducted relevant activities in this direction.

To reach all these goals, the project and its results will follow a dissemination plan through various channels once Consortium approves the contents. Key Performance Indicators (**KPIs**) will monitor the dissemination actions and channels defined in the Dissemination and Communication Plan. KPIs will include ≥ 5 publications in high-impact peer-reviewed journals (open access); ≥ 2 dissemination events (workshops (co)organized by the project); ≥ 3 different flyers & posters, and press releases; ≥ 1000 accesses to the project website & newsletters (annual). The plan will also foster the idea-to-innovation throughout the execution of the project to finally deliver: the prototype for continuous solar H_2 production.

The project results will be valuable for the regulation, certification, and standardisation of solar fuels and the social acceptability of the technology.

Innovation to the context of reference

In the metropolitan area of Messina, alongside a high potential for renewable energy (wind, solar, geothermal, tidal, etc.), there is an industrial site (Milazzo) on energy (Refinery of Milazzo and the A2A Energiefuture plant of San Filippo del Mela), in severe crisis and which must change the development model. Around 5,000 jobs (including related industries) are at risk. The revitalization of this area is a priority for the Region. The SCOOP project and CASPE centre can be crucial elements for revitalising this area through the energy transition.

In synergy with Enel Green Power, as commented above, it can be considered to use their panel to create a new factory for solar-to-hydrogen panels, which can be installed in the A2A Energiefuture plant in Milazzo (total surface is 540.000 m^2 largely by dismissed plants former dedicated to energy production) to produce green H_2 for the nearby refinery (Raffineria di Milazzo). This is an example of the possible positive synergies for industrial reconversion and, at the same time, acceleration of the transformation to a sustainable and resilient future, which can be derived from the development of the SCOOP project. UniME has direct relations with these industrial players, which makes it potentially possible to realize this proposed innovation.

This is not the only possible example of the relevance of the SCOOP project for the local industrial context of reference. Duferco Engineering, which also has one of its factories in Milazzo, has involved UniME in the project to reduce the carbon footprint by using a mixture of H_2 and natural gas in its plant. The H_2 is planned to be produced by electrolysis. Still, the company is also interested in the PV sector; thus, using modified PV units that can directly produce H_2 is highly interesting.

These are two specific examples. The *Solar Fuel Hub*, a lasting result of the SCOOP project, can thus become the enabling structure of the transformation that combines knowledge resources with the needs of society and industry to accelerate innovation mechanisms. This is the overarching and long-term goal UniME has set for itself and the groups operating in the area of renewable energy and solutions for green H_2. Companies and Institutions will collaborate in research to produce knowledge and develop concrete applications in the ecological and circular transition multidisciplinary fields.

The project innovation to booster companies such as *Enel Green Energy* was mentioned above. More than 50 startups, including Nemesys, Solid Power, Enapter, CTS and Test Energy, are potentially interested in the project results, together with large companies such as Snam, NextChem/Sapio, Loccioni. The PI and CASPE centre have relations with several of them and other cutting-edge national and international research centres – like CNR, FBK, ENEA, and RINA – that can collaborate to develop the technology further.

SECTION 4

Chronoprogramme

The project's timing (chronoprogramme) was presented in the Pert and Gantt charts (Figure 6 and Figure 12, respectively). It is a four years project for the necessity to initially improve further the electrodes and cells (around the 1st year of the project), scale-up them, manufacture and operate the prototype unit (the core of the project, from 2nd to 4th year), validate the prototype and perform techno-economic (TEA) and LCA assessment (last year), and implement the *Solar Fuel Hu*b and use it to promote and showcase the technology (last year). These activities thus correspond to three blocks of activities along the lines indicated in the call (see Figure 12):

- a first non-predominant stage of fundamental research during the first year of the project
- a predominant stage of industrial research up to prototype planned from around the start of the 2nd year up to the end of the project
- a non-predominant set of experimental development activities in the last year of the project.

The details of the human resources for the various WPs and tasks are indicated in Figure 12 and Tables 1 & 2. The core activities (industrial research) will require around 124 PMs, with the participation of around 7-10 UniME permanent personnel and 3-6 between post-doc and PhDs. The fundamental research and experimental development will cumulatively require about 35% of total PMs personnel.

A series of deliverables to monitor the progress of the activities and intermediate and final milestones are planned, the latter described in the following sections. Figure 16 summarizes the deliverables and milestones for the SCOOP project.

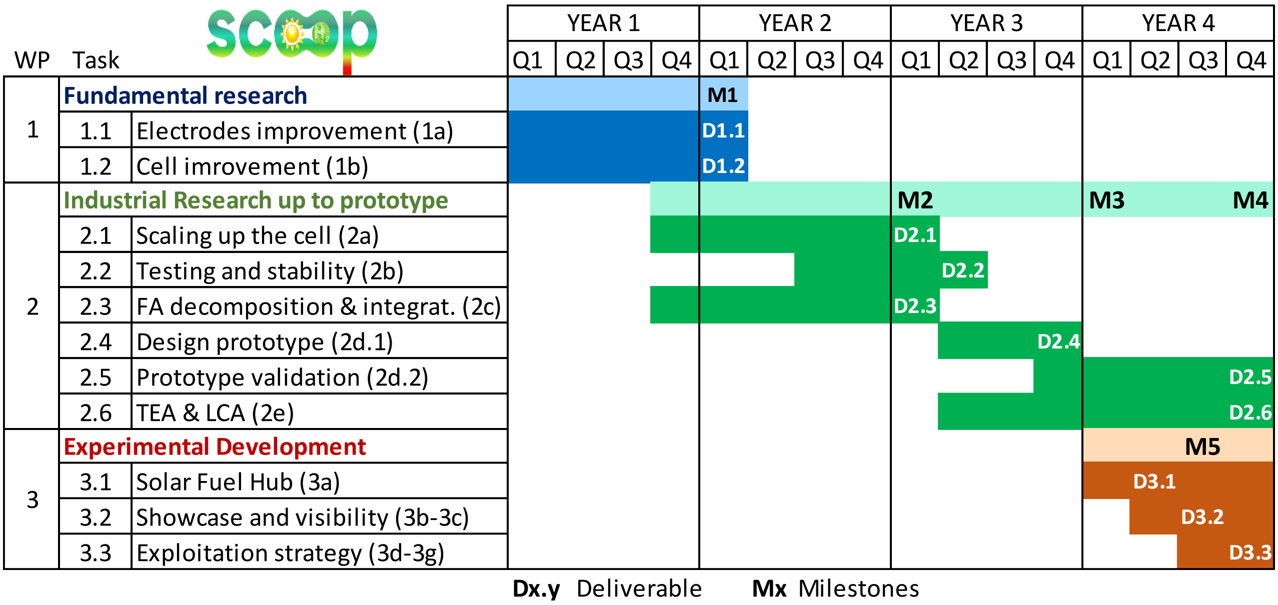


Figure 16 Gantt chart of the SCOOP project with indications of the deliverables (D) and Milestones (M).

Table 5 details the planned deliverables (**D**), while the following section will describe milestones (M).

Table 5 Description of the deliverables (**D**) for the project SCOOP (**KPI**: key performance indicators, **M** months at which the deliverable is expected)

Deliverables	*Description*
D1.1	Identified within M14 at least a cathode and anode optimized preparation suitable for scaling and that meets the KPI project indicators
D1.2	Identified within M15 an optimized AL-type cell design and configuration suitable for scaling that meets the KPI project indicators
D2.1	Completed within M25 the scaling of the AL-type unit to a size of the electrodes ≥10x10 cm
D2.2	Completed within M25 the testing of the optimized electrodes and AL-type cell to meet the KPI project indicators regarding stability
D2.3	Identified within M26 the catalyst and reactor design for the scalable FA-decomposition unit
D2.4	Completed within M36 the design of the prototype unit, including safety analysis
D2.5	Completed within M48 the validation tests (performances, stability) of the prototype unit according to KPI project indicators
D2.6	Completed within M48 the simplified TEA and LCA assessment of the technology based on prototype results
D3.1	Operative within M39, the Solar Fuel Hub
D3.2	Organization within M42 of a showcase event to present to stakeholders and the public the technology
D3.3	Prepared within M48 an exploitation strategy report for the project results

Risk evaluation and mitigation

SCOOP project is structured to minimize the risks, although remaining an ambitious project that aims to develop a non-existing technology for continuous solar H_2. It starts from TRL 3 results of a previous EU FET project (A-LEAF), although integrating them with different components to shift the objective from the conversion of CO_2 to FA to the use of the results to produce H_2 in a continuous mode (using FA as an onsite chemical storage system). In addition, there is a consolidated experience by the PI and associated team in scaling up to TRL 5-6 (in the frame of EU industrial projects) technologies which are related to this project. Thus, there is a direct experience in timing and possible issues that can occur.

Furthermore, lasting sustainability and impact are addressed by creating the Solar Fuel Hub, which will remain after the end of the project and will act as a lasting element to **i**) showcase the results to stakeholders and the public, **ii**) continue experimentation of the prototype, and **iii**) be a physical space for developing applications of the technology in interaction with companies.

As commented before, PI and the associated team already have a solid network of interaction with companies at local, national and international levels and with science and technology providers, which may help develop and consolidate the project results.

Table 6 reports a more specific analysis of critical risks for implementation and the proposed risk-mitigation measures. A *general risk* is that due to the reduction of the total budget for the project, around 24%, a cut in the personnel and other costs has been necessary while maintaining all the commitments (deliverables, timescale, milestones, etc.) of the original proposal. For example, the PMs have been reduced from 284 PMs (original proposal) to 190 PMs (revised after negotiation). This fact determines a lack of sufficient human resources to perform all the planned activities.

Table 6. Critical risks for the implementation of the proposed risk-mitigation measures. **L**: likelihood and **S**: severity, the following number indicates the level of severity: 1 - Low, 2 - Medium and 3 - High)

Description of risk	WP	Proposed risk-mitigation measures
Electrodes do not reach project targets on a lab scale. L1, S2	1	Increase effort on electrodes modification; analyse the factors limiting performances; modify the cell to limit losses; use the experience in other projects
Cell (lab-scale) does not reach project targets. L1; S2	1	Intensity analysis of the factors limiting performances; use of additional engineering competencies; revised design
Loss in the performances in scaled-up electrodes. L2, S2	2	Improve the effort in scaling up; use alternative preparation; characterize electrodes to identify the reasons; use other expertises
Cell design does not allow scale-up L1; S1	2	Revise design to improve easier scale-up; use the experience of a network of cooperation; improve effort on cell engineering
Up-scaled photovoltaic modules do not deliver sufficient voltage at high solar conv. efficiency L1, S2	2	Optimize contact and interconnection technologies by closer cooperation with suppliers of these modules; consult other PV suppliers
Catalysts and reactor for FA decomposition do deliver enough rate for integration within the upscaled process L2, S2	2	Intensity analysis of the factors limiting performances; use of additional engineering and catalytic competencies; revised design
Insufficient performance and up-scaling of the prototype L2; S2	2	Constant monitoring to identify critical elements and increase efforts where needed; go back to cell/electrode design
Stability is not enough in continuous operations, and issues in recycling CO_2 L2; S2	2	Intensify activities to improve cell/electrode design and characteristics, better use internal and external expertise, and component analysis to identify critical elements;
Delay in equipment procurement, subsequent delays in erection and commission, prototype installation L1, S 22	2	Early identification of delays and quick communication with the suppliers to search for possible solutions
Impact, performances and KPIs (technical, environmental or economic) do not comply with the project's objectives. L2, S2	2	Constant monitoring during the project to early identify key elements that might cause problems, evaluate alternative strategies to reach the expected targets, and early screening analyses to flag obstacles
High CAPEX, OPEX and COP costs of SCOOP technology L1, S2	2	Optimize design and components, increase electrode productivity, minimize downstream operations
Novel technologies better than those targeted L1, S1	3	Monitor technology scenario; early introduction of changes in planned activities to account for SoA
D&C activities not effective L1, S1	3	Adopt measures and indicators to monitor the D&C activities; periodic review & updating of D&C plans
"Management Risk" – if tasks are not scheduled properly L1, S1	3	Stimulate group leader responsibility; analyse to correct deviations; intensify project monitoring.

Key performances indicators (KPI)

We could identify two series of KPIs concerning **i**) the scientific and technology development within the project and **ii**) the dissemination and communication activities to strengthen the visibility and impact of the project. They are described in Table 7 and Table 8, respectively.

Table 7 KPI for the scientific and technology development within the project

KPI	*Ref. WP*	*Description*
KPI-1	WP1	*Electrode and lab-scale cell*: (i) based on earth-abundant element, (ii) Faradaic carbon selectivity in cathode > 98%; (iii) stability in at least 30h operations (less than 5% lowering of the current density); (iv) current density over 20 mA·cm^{-2}; (v) ratio of faradaic selectivities to FA and H_2 at least over 1.4
KPI-2	WP2	*Scalability*: (i) reliable production of electrodes with size at least 10x10cm using industrial-relevant preparation methodologies; (ii) loss of performances to lab-scale electrodes less than 10%; (iii) stability of operations using recycled CO_2 from FA decomposition; (iv) use of optimized, low-cost PV modules
KPI-3	WP2	*Operability*: (i) design a full system prototype for continuous of H_2 at least 20 L_{NTP} of H_2 per hour and m^2 of PV panel, (ii) stable operations for at least 30h of the whole system with CO_2 recycle from FA decomposition; (iii) operability with continuous or on-demand modes.
KPI-4	WP2	*TEA & LCA*: (i) estimated costs of H_2 production lower than the reference case (combination of H_2 electrolysis with electrical energy produced by PV and state-of-the-art storage of H_2); (ii) lower CO_2 emissions per kg H_2 than the reference case (state-of-the-art electrolysis using electrical energy with the current average share of renewable component)

Table 8 KPI for the dissemination and communication activities within the project

KPI	*Ref. WP*	*Description*
KPI-5	WP3	*Dissemination*: (i) ≥ 5 publications in high-impact peer-reviewed journals (open access), (ii) ≥ 2 dissemination events (workshops (co)organized by the project); (iii) at least 3 open days to show to the public and stakeholders the results of the project
KPI-6	WP3	*Communication*: (i) 3 different flyers & posters, and press releases; (ii) ≥ 1000 accesses to the project website & newsletters (annual)

Objectives and results: Intermediate Milestones

As outlined in Figure 16, there are two intermediate objectives (milestones), which should be met for the midterm of the project (after the second year, beginning the third year):

- **M1**, associated with WP1, whose objective is to have developed optimized electrodes and AL-type cell design at lab-scale (electrodes size in the 5-10 cm^{-2} range) which meet the KPI-1
- **M2**, associated with WP2, whose objective is to have scaled the electrode preparation and cell, as well as have defined the catalysts and optimal conditions of operation for the FA decomposition unit, which meet KPI-2

Reaching these intermediate objectives (milestones) requires to achieve

- for M1 it should achieve the deliverables D1.1. and D1.2, with the associated KPI-1
- for M2 it should be achieved the deliverables D2.1, D2.2 abd D2.3, with the associated KPI-2

Objectives and results: Final Milestones

As outlined in Figure 16, there are three final project objectives (milestones), e.g. at the end of the 4th year of the project:

- **M3**, associated with WP2. The objective is to have completed the design and manufacture of the prototype unit which meets KPI-3
- **M4**, associated with WP2. The objective is to have validated the prototype in terms of

performance and stability (meet KPI-3) and TEA & LCA assessment (meet KPI-4)

- M5, associated with WP3. The objective is to create and make operative the Solar fuel Hub and its use for dissemination and communication activities (meet KPI-5 and KPI-6), as well as to showcase the results of the project, particularly the prototype, to the public and stakeholders, to prepare a lasting strategic planning for project results exploitation.

Reaching these final objectives (milestones) requires to achieve

- for M3 it should be achieved the deliverables D2.4, with the associated KPI-3
- for M5 it should be achieved the deliverables D2.5 and D2.6, with the associated KPI-4
- for M6 it should be achieved the deliverables D3.1-D3.3, with the associated KPI-5 and KPI-6

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Document signatures

Date, 06 Feb. 2024

The Principal Investigator
Prof.sa Siglinda Perathoner

Ministero dell'Università e della Ricerca

Segretariato Generale
Direzione generale della ricerca

Allegato B

Codice	FISA2022-00277
Area	Energy
Acronimo	SCOOP
Principal Investigator	Siglinda Perathoner

Ambito di Attività	**Costi**		**Agevolazioni**	
	(€)	***(%)***	***(€)***	***Intensità di aiuto (%)***
Ricerca Fondamentale	290.749,02 €	15%	290.749,02 €	100%
Ricerca Industriale	1.416.018,56 €	75%	1.416.018,56 €	100%
Sviluppo Sperimentale	189.811,07 €	10%	189.811,07 €	100%
Totale	**1.896.578,66 €**	**100%**	**1.896.578,66 €**	

Soggetto	**Codice Fiscale**	**Ruolo**	**Tipologia di Soggetto**	**Ambito di attività**						**Totale**	
				Ricerca Fondamentale		**Ricerca Industriale**		**Sviluppo Sperimentale**			
				Costo (€)	**Agevolazione (€)**	**Costo (€)**	**Agevolazione (€)**	**Costo (€)**	**Agevolazione (€)**	**Costo (€)**	**Agevolazione (€)**
Università degli Stuidi di Messina	80004070837	***HI/AI***	***Non destinatario di Aiuti di Stato***	290.749,02 €	290.749,02 €	1.416.018,56 €	1.416.018,56 €	189.811,07 €	189.811,07 €	1.896.578,66 €	1.896.578,66 €
			Totale	**290.749,02 €**	**290.749,02 €**	**1.416.018,56 €**	**1.416.018,56 €**	**189.811,07 €**	**189.811,07 €**	**1.896.578,66 €**	**1.896.578,66 €**

Ministero dell'Università e della Ricerca

Segretariato Generale
Direzione generale della ricerca

Allegato C

Cronoprogramma di attuazione

Ambito di Attività	*Descrizione Obiettivo Ambito di Attività*		giu-24	dic-24	gen-25	ago-25	dic-25	giu-26	dic-26	mar-27	giu-25	set-27	dic-27	may-28		*Costo Ambito di Attività (€)*	*Agevolazioni (€)*
		T0	**1**	**7**	**7**	**15**	**18**	**27**	**30**	**33**	**36**	**39**	**42**	**48**	**TF**		
Ricerca Fondamentale	Ottimizzazione degli elettrodi e cella															290.749,02 €	290.749,02 €
Ricerca Industriale	Sviluppo, realizzazione, valutazione e testing unità prototipo															1.416.018,56 €	1.416.018,56 €
Sviluppo Sperimentale	Showcase tecnologia, Solar Fuel Hub, Dissem e Visibilità, Piano sfrutt risultati															189.811,07 €	189.811,07 €
																1.896.578,66 €	**1.896.578,66 €**

	T0	1	7	7	15	18	27	30	33	36	39	42	48	TF	
Cronoprogramma delle agevolazioni															**Totale**
Cronoprogramma delle rendicontazioni			125.584,22 €		286.216,98 €		215.465,36 €		529.866,20 €		516.071,50 €		223.374,40 €		1.896.578,66 €
di cui Ricerca Fondamentale			125.584,22 €		165.164,80 €										290.749,02 €
di cui Ricerca Industriale					121.052,18 €		215.465,36 €		529.866,20 €		414.306,33 €		135.328,50 €		1.416.018,57 €
di cui Sviluppo Sperimentale											101.765,18 €		88.045,90 €		189.811,07 €
Piano delle erogazioni	**189.657,87 €**		**222.143,34 €**		**215.465,36 €**		**529.866,20 €**		**516.071,50 €**		**33.716,53 €**			**189.657,87 €**	**1.896.578,66 €**

Ministero dell'Università e della Ricerca

Segretariato Generale
Direzione generale della ricerca

Avviso n. 1405 del 13 settembre 2022 – Avviso pubblico "*finalizzato al finanziamento di proposte progettuali con le risorse del FISA – Fondo Italiano per le Scienze Applicate, per l'anno 2022*"

Allegato D al Decreto di Concessione

ART. 1
Oggetto

1. Il presente Disciplinare, da perfezionare mediante la sottoscrizione dell'Atto d'Obbligo da parte dei Soggetti beneficiari, regola i rapporti tra il MUR e i predetti Soggetti, nonché i relativi termini e condizioni, le modalità di attuazione e gli obblighi di rendicontazione del Progetto identificato con codice FISA-2022-00277 dal titolo "*SCOOP-Novel Solar cells for solar-to-hydrogen COntinuOus Production*".

ART. 2
Termini di attuazione del Progetto, durata e importo del finanziamento

1. I Soggetti beneficiari si obbligano a svolgere le attività definite nel Progetto finale, come risultante in esito alla Fase negoziale, e nel relativo Capitolato Tecnico e ad attuare gli obiettivi previsti secondo le modalità, i termini e le condizioni stabilite dalla legge, dai regolamenti, dagli atti e provvedimenti ministeriali, dagli allegati al Decreto di Concessione, nonché dal presente Disciplinare.
2. La durata di realizzazione del Progetto è fissata dal Cronoprogramma, Allegato C al Decreto di Concessione a decorrere dalla data indicata all'interno dello stesso.
3. Il MUR può valutare ed autorizzare una proroga rispetto alla durata prevista, previa tempestiva comunicazione ed in caso di comprovata necessità per il completamento delle attività.
4. L'importo del finanziamento, nella forma del contributo alla spesa a valere sul Fondo Italiano per le Scienze Applicate (FISA) 2022 (*l'"agevolazione*"), è indicato all'art. 2, comma 1 del Decreto di Concessione.

ART. 3
Obblighi dei Soggetti beneficiari

I Soggetti beneficiari si obbligano a:

a) impegnarsi ad eseguire il Progetto nei tempi, modi e forme previste dal relativo Capitolato Tecnico e dagli ulteriori atti e provvedimenti, nonché, dalla vigente normativa e nel rispetto di quanto contenuto nel presente Disciplinare e con la diligenza e professionalità necessaria al raggiungimento degli obiettivi progettuali;
b) adoperarsi a collaborare ai fini del tempestivo svolgimento degli accertamenti previsti ai sensi del D.Lgs. 159/2011 e ss.mm.ii. a cura delle competenti Autorità, e di relativa acquisizione da

parte del MUR. In particolare, si applicano le disposizioni di cui agli articoli 84 e seguenti del D.Lgs. 159/2011 e ss.mm.ii.. In caso di eventuale riscontro non favorevole da parte delle competenti Autorità, il MUR provvederà all'immediata revoca delle agevolazioni concesse ai sensi del successivo art. 7 del presente Disciplinare;

c) essere in regola con gli obblighi contributivi di cui al D.U.R.C. sia in caso di istanza di pagamento dell'anticipazione sia per le successive erogazioni;

d) effettuare i controlli di gestione e i controlli amministrativo-contabili previsti dalla legislazione nazionale applicabile, per garantire la regolarità delle procedure e delle spese sostenute prima di rendicontarle al MUR;

e) produrre tutte le richieste di informazioni, di dati e di rapporti tecnici periodici disposte dal MUR;

f) comprovare, la conclusione delle Attività Progettuali, l'avvenuto conseguimento di tutti gli obiettivi di ricerca previsti dal Capitolato Tecnico e la realizzazione del Progetto, emettendo, all'Esperto Tecnico–Scientifico e all'Esperto Economico–Finanziario, una relazione tecnica relativa all'ultimo periodo di avanzamento e all'intero programma svolto, comprendente il rendiconto dei costi dell'ultimo periodo nel rispetto delle modalità indicate dal MUR;

g) consentire e favorire, in ogni fase del procedimento, lo svolgimento di tutti i controlli, ispezioni e monitoraggi disposti dal MUR, facilitando altresì le verifiche dell'Ufficio competente per i controlli del MUR, dell'Unità di Audit e di altri organismi autorizzati, che verranno effettuate anche attraverso controlli in loco presso i Soggetti attuatori pubblici delle azioni;

h) tenere a disposizione del MUR, per ulteriori 5 anni dalla data dell'ultima erogazione sul Progetto, tutta la documentazione sopra indicata;

i) assicurare il rispetto di tutte le disposizioni previste dalla normativa comunitaria e nazionale;

j) a garantire, nel caso in cui si faccia ricorso alle procedure di appalto, il rispetto di quanto previsto dal d.lgs. 36/2023 e ss.mm.ii.;

k) rispettare la normativa applicabile in materia di tracciabilità di flussi finanziari;

l) tenere specifica separata evidenza contabile desumibile da sistemi informatici che consentano di ottenere, in ogni momento, estratti riepilogativi e sinottici di tutte le movimentazioni riguardanti il Progetto, nel rispetto dell'art. 125, comma 4, lettera b), del Regolamento UE n. 1303/2013;

m) rispettare l'obbligo di indicare il CUP di cui all'Allegato E "Codici Unici di Progetto (CUP) e su tutti gli atti amministrativo/contabili relativi al progetto;

n) garantire l'utilizzo di un conto corrente dedicato necessario per l'erogazione dei pagamenti;

o) partecipare, ove richiesto, alle riunioni convocate dal MUR;

p) rispettare le prescrizioni in materia di prevenzione e repressione della corruzione e dell'illegalità nella pubblica amministrazione ai sensi della legge 6 novembre 2012, n. 190 e ss.mm.ii.;

q) rispettare le prescrizioni in materia di trasparenza amministrativa ai sensi del d.lgs. 14 marzo 2013, n. 33 e ss.mm. ii.;

r) assicurare il rispetto della normativa vigente sugli aiuti di Stato;

s) rispettare, sin da ora, tutti gli obblighi afferenti alle modalità di rendicontazione, le attività di monitoraggio, controllo, informazione e pubblicità;

t) garantire il rispetto di eventuali previsioni normative, orientamenti o istruzioni tecniche che potranno essere emanate dal MUR, anche successivamente alla pubblicazione dell'Avviso.

ART. 4
Procedura di rendicontazione dell'avanzamento degli obiettivi negli ambiti di attività e delle spese

1. La procedura di rendicontazione delle agevolazioni è espletata ai sensi del Decreto ministeriale n. 1314 del 14 dicembre 2021 e ss.mm.ii. e in base al Cronoprogramma di attuazione di cui all'Allegato C del Decreto di Concessione, e al Piano dei Costi di cui all'Allegato B del Decreto di Concessione.
2. I Soggetti beneficiari producono e trasmettono, secondo le modalità e la modulistica indicata dal MUR e mediante l'utilizzo del sistema informatico da questo adottato, la complessiva documentazione attestante le attività progettuali svolte, con particolare riferimento al conseguimento degli obiettivi, intermedi e finali, previsti dal progetto approvato.
3. I costi relativi alle spese di cui all'art. 5 comma 2 dell'Avviso sono rendicontati secondo i valori delle Unità di Costo Standard approvate dalla Commissione Europea e adottate con Decreto interministeriale MIUR-MISE prot. n. 116 del 24 gennaio 2018 e ss.mm.ii.. È ammessa la rendicontazione del costo reale esclusivamente nel caso in cui per la particolare tipologia di costo non sia disponibile un analogo valore standard.
4. Le spese incluse nelle progressive rendicontazioni presentate dai Soggetti Beneficiari sono sottoposte, alle verifiche, se del caso anche in loco da parte delle strutture deputate al controllo del MUR.

ART. 5
Procedura di pagamento ai Soggetti Beneficiari

1. La procedura di erogazione delle agevolazioni è espletata ai sensi del Decreto ministeriale n. 1314 del 14 dicembre 2021 e ss.mm.ii. e in coerenza con il Cronoprogramma di attuazione di cui all'Allegato C del Decreto di Concessione, e il Piano dei costi di cui all'Allegato B del Decreto di Concessione.
2. I Soggetti beneficiari, in esito alla fase di sottoscrizione dell'Atto d'Obbligo potranno richiedere una prima erogazione, a titolo di anticipazione, nella misura massima del 10% dell'importo agevolato. Nel caso di un Soggetto beneficiario di diritto privato l'erogazione

a titolo di anticipo dovrà essere assistita da idonea garanzia fornita da una banca o da qualunque altra istituzione finanziaria o coperta da uno strumento fornito a garanzia da un ente pubblico, o dallo Stato membro da mantenere per tutta la durata del progetto.

5. La documentazione di cui all'articolo 4, comma 2 del presente Disciplinare, attestante le attività progettuali svolte è sottoposta alla valutazione del MUR, per il tramite di organi di valutazione scientifica nominati dal CNVR nell'ambito di appositi elenchi gestiti dalla Commissione Europea, dal Ministero stesso, da altre istituzioni nazionali o eurounionali.
6. All'esito positivo delle verifiche di cui al precedente comma, il MUR, in base al conseguimento degli indicatori di avanzamento collegati agli obiettivi associati all'intervento, ed in coerenza con il Piano dei costi previsti dal Decreto di Concessione del finanziamento, dispone le erogazioni del contributo pubblico in favore dei Soggetti beneficiari, sino al massimo del 90% dell'agevolazione complessivamente approvata.
7. La documentazione amministrativo – contabile relativa alle spese sostenute è sottoposta alle valutazioni del MUR, per il tramite dell'Agenzia nazionale per l'attrazione degli investimenti e lo sviluppo d'impresa Spa – Invitalia - in attuazione della Legge 30 dicembre 2020, n. 178 art. 1 comma 550, di banche e società finanziarie, ovvero di altri soggetti qualificati, dotati di comprovata competenza, professionalità e strumenti tecnici adeguati, individuati nel rispetto del diritto applicabile.
8. All'esito delle verifiche di cui al precedente comma, il MUR accerta il contributo pubblico maturato in relazione alle spese ammissibili, rispetto alle erogazioni precedentemente disposte, adottando, se necessario, le relative procedure compensative all'atto dei successivi trasferimenti ai fini del riallineamento contabile.
9. L'erogazione finale è disposta a conclusione del progetto, sulla base dei costi effettivamente sostenuti e del conseguimento degli obiettivi fissati e positivamente valutati secondo la procedura descritta nell'art. 12 dell'Avviso. Qualora l'ammontare delle erogazioni precedentemente disposte sia superiore all'ammontare del contributo pubblico maturato in relazione alle spese ammissibili, è disposto il recupero della differenza.
10. In caso di mancata restituzione degli importi per i quali è stato disposto il recupero, il MUR adotta ogni utile determinazione a tutela dell'interesse pubblico, anche mediante:
    a) il fermo amministrativo ai sensi dell'articolo 69 del R.D. 18 novembre 1923 n. 2440 e ss.mm.ii., a salvaguardia dell'eventuale compensazione mediante somme a favore dei Soggetti beneficiari e/o dei soggetti esecutori maturate su altri progetti finanziati o ad altro titolo presso il MUR o altra Amministrazione;
    b) la revoca delle agevolazioni e recupero delle somme erogate attivando le procedure di iscrizione al ruolo previste dall'articolo 6, comma 6-bis del Capo IV del D.L. 14 marzo 2005, n. 35 convertito con L. 14 maggio 2005 n. 80.
11. Ove il MUR ricorra al recupero delle medesime somme dovute da un soggetto di diritto pubblico, restano ferme le disposizioni vigenti in materia di credito e debito tra Amministrazioni.

ART. 6
Varianti progettuali

1. Variazioni soggettive, riguardanti operazioni societarie dei beneficiari, e variazioni oggettive, riguardanti il piano dei costi e delle attività, così come presentato in fase di domanda ed approvato in fase di ammissione, sono ammissibili ma devono essere tempestivamente e obbligatoriamente comunicate al Ministero. Le medesime variazioni non richiedono da parte dei soggetti attuatori approvazione preventiva da parte del MUR, a condizione che non incidano sugli aspetti qualitativi ed economico-finanziari oggetto di valutazione ex ante, non alterino gli aspetti esecutivi degli interventi definiti nella fase negoziale e non abbiano impatto rispetto alle finalità dell'intervento così come definito nell'Avviso e al conseguimento degli obiettivi negli ambiti di attività, intermedi e finali, connessi all'esecuzione del Progetto.
2. Ogni eventuale variazione che ecceda i limiti e le condizioni previste nel precedente comma 1 dovrà essere sottoposta alla preventiva approvazione da parte del Ministero.
3. Le variazioni intervenute nel corso del progetto sono oggetto di Decreto ricognitivo finale, da redigersi a conclusione del progetto e preliminare all'erogazione del saldo finale.
4. Fatto salvo quanto previsto al comma 1, qualora, nel corso delle verifiche di cui al precedente art. 5, commi 3 e 5, emergano significative deviazioni rispetto ad uno dei seguenti elementi riportati nel Decreto di Concessione:
   a) finalità dell'intervento;
   b) raggiungimento degli obiettivi, intermedi e finali;
   c) cronoprogramma di attuazione;
   d) volume di spesa;
   il MUR, anche mediante il supporto di organi di supervisione scientifica, può richiedere ai Soggetti beneficiari l'adozione di misure correttive e revisioni complessive di Progetto, anche in termini di rideterminazione dei costi complessivi dell'intervento.
5. Le misure correttive e revisioni complessive di Progetto di cui al precedente comma sono valutate dal MUR, anche mediante il supporto di organi di supervisione scientifica e approvate mediante apposito provvedimento Ministeriale, a modifica del Decreto di Concessione e dei pertinenti allegati.
6. Qualora la procedura di cui al precedente comma non consenta comunque il corretto e completo svolgimento del Progetto finanziato, il Ministero adotta le determinazioni di cui all'articolo 7 del presente Disciplinare.
7. Le variazioni e le modifiche di cui ai precedenti commi non comportano alcuna revisione del presente Disciplinare.

ART. 7
Morosità, Revoca e Interruzione

1. Sono applicate, ove pertinenti, le disposizioni procedurali di cui all'art. 17 del Decreto Ministeriale n. 1314 del 14 dicembre 2021 e ss.mm.ii.

ART. 8
Rettifiche finanziarie

1. Ogni difformità rilevata nella regolarità della spesa, prima o dopo l'erogazione del contributo pubblico in favore dei Soggetti Beneficiari, dovrà essere immediatamente rettificata e gli importi eventualmente corrisposti dovranno essere recuperati.
2. A tal fine i Soggetti Beneficiari si impegnano, a restituire le somme indebitamente corrisposte. I Soggetti Beneficiari sono obbligati a fornire tempestivamente ogni informazione in merito a errori od omissioni che possano dar luogo a riduzione o revoca del contributo.

ART. 9
Risoluzione di controversie

1. Il presente Disciplinare è regolato dalla legge italiana. I Soggetti Beneficiari, mediante la sottoscrizione dell'Atto d'Obbligo, accettano che qualsiasi controversia, in merito all'interpretazione, esecuzione, validità o efficacia, è di competenza esclusiva del Foro di Roma.

ART. 10
Comunicazioni e scambio di informazioni

1. Ai fini della digitalizzazione dell'intero ciclo di vita del progetto, tutte le comunicazioni con il MUR devono avvenire per posta elettronica istituzionale o posta elettronica certificata, ai sensi del d.lgs. n. 82/2005, o altre modalità telematiche successivamente indicate dal MUR.

ART. 11
Efficacia

1. L'efficacia del presente Disciplinare, da perfezionare mediante la sottoscrizione dell'Atto d'Obbligo da parte dei Soggetti Beneficiari, decorre dalla data di acquisizione da parte del MUR dell'Atto d'Obbligo.