



Project No. 101046294

Complex chemical reaction networks for breakthrough scalable reservoir computing

Deliverable 4.1

CORENET website

WP 4 – Communication, Dissemination and Exploitation

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Abstract

The brain is the world's most amazing computer and it runs entirely on chemical reactions. The vision of CORENET is to construct brain-mimicking computing devices that utilise networks of chemical reactions as molecular information processing systems. To achieve this vision, we will implement reservoir computing (RC) on microfluidic chips using chemical reaction networks (CRNs) that convert input feedstock molecules and environmental conditions into a pattern of product molecules. This pattern can be monitored on a chip using a combination of high-throughput mass spectrometry analysis, algorithmic cheminformatics and AI tools. CORENET will generate a breakthrough in highly scalable and functional chemical RC by integrating our partners' new knowledge and state-of-the-art methodologies in systems and analytical chemistry, microfluidics, cheminformatics and machine learning. CORENET will produce microfluidic chip devices that perform high-level computing with molecules, synthesising and analysing a pattern of output molecules in situ. This molecule-based computing power enables truly sustainable AI and speaks the language of living systems, which constantly process information about their molecular environment. Future applications of our chemical RC system lie in implantable devices, brain-machine interfaces and personalised medicine. CORENET brings together 4 leading scientists with complimentary expertise that covers all fundamental aspects of this project. Their expertise is combined with the world-class knowledge in AI/ML modelling of a high-tech global industry partner with unique research and computing infrastructure, while an SME specialised in the communication and dissemination of results will ensure maximised impact. Our highly interdisciplinary team will generate new scientific knowledge and breakthrough technologies to achieve essential priorities for Europe's future and its support to the UN Sustainable Development Goals.

Revision history

Author(s)	Description	Date
Sara Rodriguez, Anna Dovha (accelCH)	Draft version	12/05/2022
Andres de la Escosura (UAM), Wilhelm Huck (SRU)	Revision	17/05/2022
Anna Dovha (accelCH)	Final version	30/05/2022

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Partner short names

UAM	Universidad Autónoma de Madrid
SRU	Stichting Radboud Universiteit
IBM	IBM Research
CSIC	Agencia Estatal Consejo Superior de Investigaciones Científicas
SDU	Syddansk Universitet
accelCH	accelopment Schweiz AG

Abbreviations

D	Deliverable
EC	European Commission
EU	European Union
HEU	Horizon Europe
M	Month
MS	Milestone
WP	Work Package

Executive summary

This deliverable is part of the Work Package (WP) 4, task 4.2: “Cross-media communication”. It refers to the subtask of reaching a broad audience, including academics, industry representatives, school kids and the general public through CORENET communication activities, which range from online and in-person to written and audio-visual.

The website serves as the main source of information about CORENET, with up-to-date content relevant to the project, targeting different audiences. This deliverable reports the main objectives and strategy for maintaining the website, as well as provides detailed information on the structure, technical implementation, and outlook. The project website serves as a flexible tool that allows the CORENET consortium to raise awareness of the project and to provide up-to-date, consistent, and complete information to its various stakeholders.

1 Key facts

The CORENET website is key to raise awareness on the project's achievements, as well as function as the central online portal to disseminate its results to the scientific community and communicate outcomes to the general public and wider non-expert audiences.

- Website address: <https://corenet-horizon.eu/>
- The website first launched on 12th May 2022
- accelCH created and currently maintains the website using WordPress
- The CORENET website is securely hosted on accelCH's webserver.

2 Objectives

The main objective of this deliverable is the creation of a state-of-the art and user-friendly website for the CORENET project. The CORENET website aims to:

- Increase the awareness of the CORENET project and its research areas,
- Highlight the work of the consortium partners,
- Document the progress of the project and inform our target groups of results and outcomes,
- Become a platform to inform and promote planned activities to target groups,
- Recruit new researchers in various areas through the open positions portal,
- Support the visual identity of the project,
- Increase the project's impact and support our open science policy by making public reports and publications accessible.

Not only to be used as a source for information, the CORENET website also aims to become an interactive platform for exchange with our various stakeholder groups, including industry, academia and the general public. In order to do so, the website includes continuously updated engaging audio-visual materials that clearly and effectively communicate the various components of the CORENET project.

3 Strategy

As the hub for CORENET, the project website will provide information for all stakeholder groups on the partners involved in the project, on the technological and scientific details behind the research being conducted, as well as on all updates concerning the project's progress, key achievements and events.

The CORENET website aims to keep all stakeholders involved and interested in the project throughout its duration. To fulfil this objective, the project's newest results will be communicated promptly and regularly through the website and connected social media channels, news and events will be promoted timely and engagement opportunities will be included when possible, such as registration functions, feedback forms or interactive audio-visual materials.

Functional at its core, the CORENET website has been designed to be user friendly and intuitive to use. Furthermore, we have expected stakeholders to access the website in different ways. By including a responsive design, the interface adapts when viewed on a phone or tablet, making it easier to navigate on a small screen and guaranteeing convenient access to the site regardless of the device used.

4 Technical implementation

Maintained by a team with extensive experience on website development and design, the CORENET website has been created with easy functionality and upkeep so all partners can be involved if they wish it.



Figure 1: WordPress logo

4.1 WordPress

We have used the Content Management System (CMS) [WordPress](#) with the website builder [Elementor](#) to create the CORENET website. WordPress offers a high degree of flexibility and customizability so that the design, layout and functionality of the website can evolve throughout the project. The user-friendly interface facilitates efficient maintenance, and the integration of plugins also expands the website functionality even further. Another advantage of WordPress is the generally high Google search engine ranking due to the loading speed and responsive design, which adapts the website to the screen sizes of all device types.

4.2 Theme

The theme has been customised and adjusted by accelCH, following the project's visual identity. The project's visual identity has been defined, which includes the font Montserrat and Roboto used in different sizes for titles and body text to enhance the lecture flow. Headers, buttons and links are displayed in the CORENET colours, namely bright green, light blue and magenta, which redirect the user to a new site with complementary information. The text colour was set to dark grey to enhance readability.

4.3 Images and graphics

To make the website more appealing, pictures and graphics have been used to illustrate the information. This includes the use of logos for partner organisations, photos of supervisors for their profiles. The graphics used on the website will be continuously updated as results are achieved and are obtained from various beneficiaries or explicitly created for use within the CORENET project (see Figure 2).

IBM Research

IBM Research Europe — Zurich

IBM has maintained a research laboratory in Switzerland since 1956. As the European branch of IBM Research, the mission of IBM Research Europe — Zurich (in addition to pursuing cutting-edge research for tomorrow's information technology) is to cultivate close relationships with academic and industrial partners, be one of the premier places to work for world-class researchers, to promote women in IT and science, and to help drive Europe's innovation agenda. The IBM partners brings the needed expertise in silicon manufacturing and AI/Machine Learning modelling for materials/chemistry, with trained experts that understand both data science and physics/chemistry experimentation and analytics, as well as their cutting-edge **NANOTECHNOLOGY CENTER**.



Dr. Emanuel Lörtscher

Figure 2: Example of a partner profile on the CORENET website

5 Structure

The website is currently structured as described in the following sub-sections, in line with the strategy, aims and objectives described above. However, this structure and the individual web pages are subject to change over time and will be adapted as the project develops, notably to build the Results page.

The main navigation menu allows the viewer to easily reach the key pages of the website, currently including “Home”, “Research and Innovation”, “Partners”, “Results” and “News”. The EU flag and acknowledgement both are displayed in the footers throughout all pages of the site, which also includes the copyright and links to “Contact” and “Privacy Policy”.

5.1 Homepage

The [Homepage](#) is the landing page for first-time access to the website through entering the URL (URL in an internet browser (e.g. Chrome), a search engine (e.g. Google), or through a link on a different website (e.g. partner websites) (see Figure 3). When browsing through the CORENET website, users can easily return to the homepage by clicking on the CORENET logo, as is common practice for many modern websites (see Figure 4).

The landing page layout is divided into sections with different content:

- Latest news piece teaser
- Feature of “Research and Innovation” and “Partners” pages
- Aim of CORENET description
- Feature of “Core”, “Open Positions” and “Work Plan”



The screenshot shows the homepage layout of the CORENET website. At the top, there is a navigation menu with links for Project, Research and Innovation, Partners, Results, News, and Cookie policy. The main header features the CORENET logo and the tagline "Complex chemical reaction networks for breakthrough scalable reservoir computing". Below this, there is a section titled "The first CORENET General Assembly" with a "Read the news" link. The main content area is divided into two columns: "RESEARCH AND INNOVATION" and "PARTNERS", each with a brief description and a "Read more" link. A central section titled "WHAT IS THE AIM OF CORENET?" explains the project's goal. Below this, there are three circular icons representing "CORE", "OPEN POSITIONS", and "WORK PLAN", each with a short description. The footer includes the European Union logo and a statement of funding, along with a quote about the consortium's interdisciplinary nature and a "William Hall CORENET Partner" logo.

Figure 3: [Homepage](#) view of the website

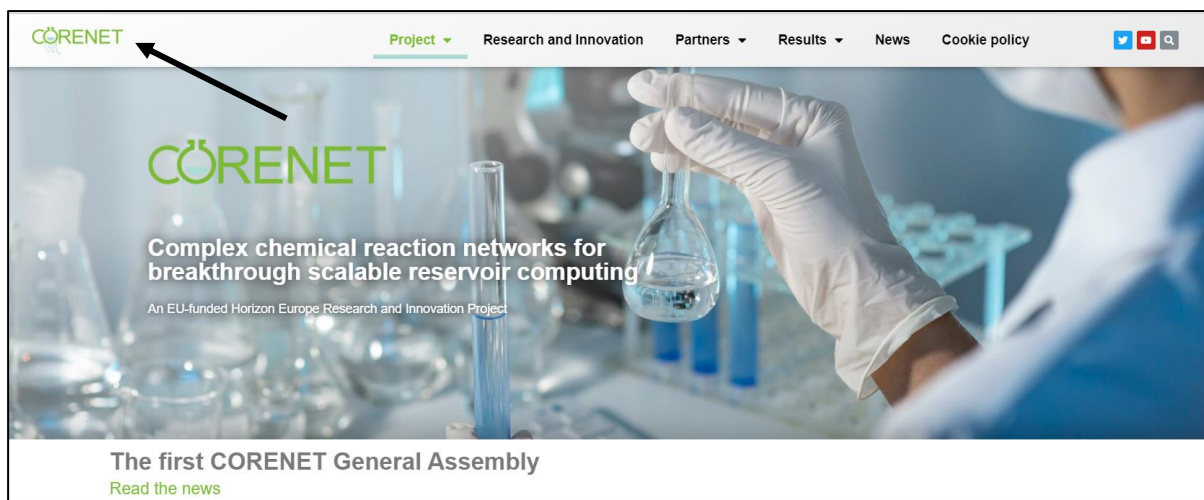
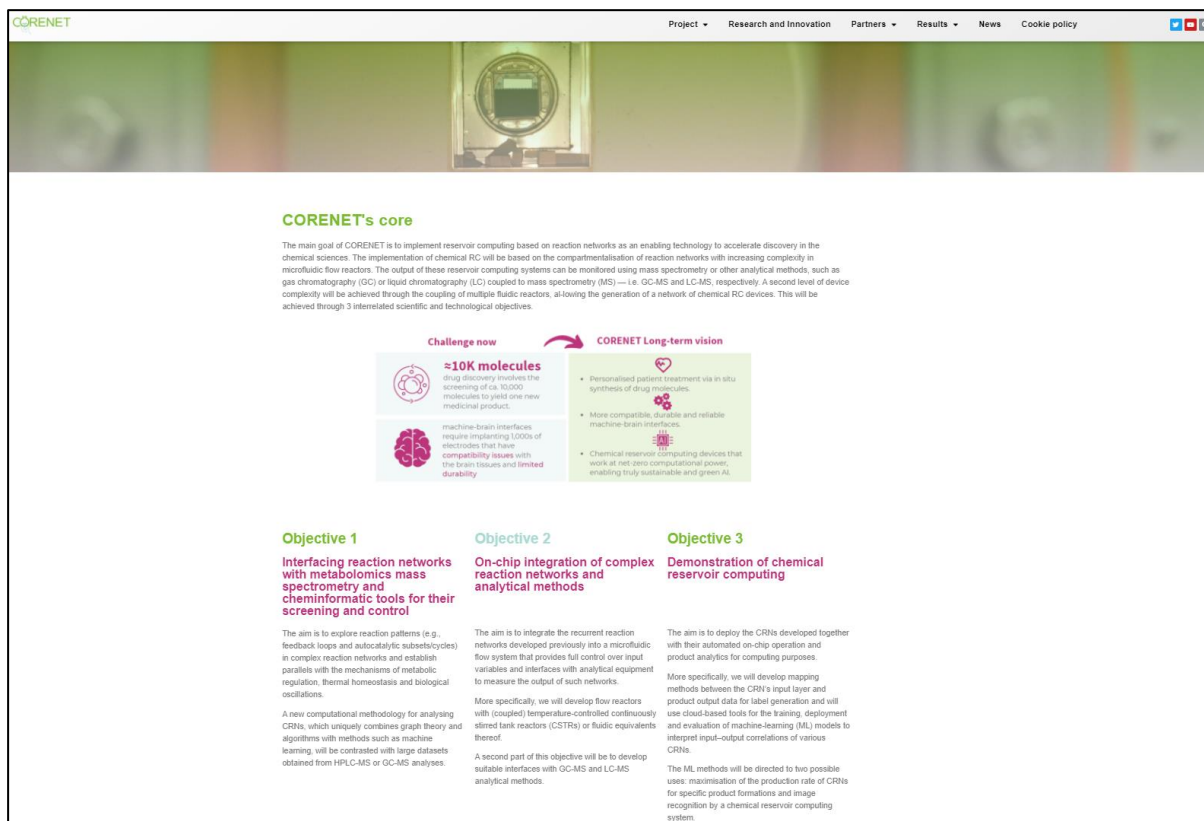


Figure 4: Overview of the CORENET logo button which users can use to return to the Homepage

5.2 CORENET's Core and Work Plan

These subpages serve as an introduction to the CORENET project, its challenges and objectives (see Figure 5 & 6). It also includes insights on how European research projects work and the intricacies between the different work packages.



CORENET's core

The main goal of CORENET is to implement reservoir computing based on reaction networks as an enabling technology to accelerate discovery in the chemical sciences. The implementation of chemical RC will be based on the compartmentalisation of reaction networks with increasing complexity in microfluidic flow reactors. The output of these reservoir computing systems can be monitored using mass spectrometry or other analytical methods, such as gas chromatography (GC) or liquid chromatography (LC) coupled to mass spectrometry (MS) — i.e. GC-MS and LC-MS, respectively. A second level of device complexity will be achieved through the coupling of multiple fluidic reactors, allowing the generation of a network of chemical RC devices. This will be achieved through 3 interrelated scientific and technological objectives.

Challenge now

- ≈10K molecules drug discovery involves the screening of ca. 10,000 molecules to yield one new medicinal product.
- machine-brain interfaces require implanting 1000s of electrodes that have compatibility issues with the brain tissues and limited durability.

CORENET Long-term vision

- Personalised patient treatment via in situ synthesis of drug molecules.
- More compatible, durable and reliable machine-brain interfaces.
- Chemical reservoir computing devices that work at net-zero computational power, enabling truly sustainable and green AI.

Objective 1
Interfacing reaction networks with metabolomics mass spectrometry and cheminformatic tools for their screening and control

The aim is to explore reaction patterns (e.g., feedback loops and autocatalytic subsets/cycles) in complex reaction networks and establish parallels with the mechanisms of metabolic regulation, thermal homeostasis and biological oscillations.

A new computational methodology for analysing CRNs, which uniquely combines graph theory and algorithms with methods such as machine learning, will be contrasted with large datasets obtained from HPLC-MS or GC-MS analyses.

Objective 2
On-chip integration of complex reaction networks and analytical methods

The aim is to integrate the recurrent reaction networks developed previously into a microfluidic flow system that provides full control over input variables and interfaces with analytical equipment to measure the output of such networks.

More specifically, we will develop flow reactors with (coupled) temperature-controlled continuously stirred tank reactors (CSTRs) or fluidic equivalents thereof.

A second part of this objective will be to develop suitable interfaces with GC-MS and LC-MS analytical methods.

Objective 3
Demonstration of chemical reservoir computing

The aim is to deploy the CRNs developed together with their automated on-chip operation and product analytics for computing purposes.

More specifically, we will develop mapping methods between the CRN's input layer and product output data for label generation and will use cloud-based tools for the training, deployment and evaluation of machine-learning (ML) models to interpret input-output correlations of various CRNs.

The ML methods will be directed to two possible uses: maximisation of the production rate of CRNs for specific product formations and image recognition by a chemical reservoir computing system.

Figure 5: Overview of the 'CORENET's Core' page accessible in the submenu of the key menu 'Home'

CORENET's work plan

The CORENET research methodology follows a modular and parallel approach.

The first three scientific work packages contain the following:

- WP1 lays the foundation of the Recurrent Neural Networks
- WP2 enables the on-chip integration of the RNNs. Their initial results will be required for
- WP3 to build up the CRN.

The two non-scientific Work Packages, WP4 and WP5, will run in parallel from the whole project's duration.

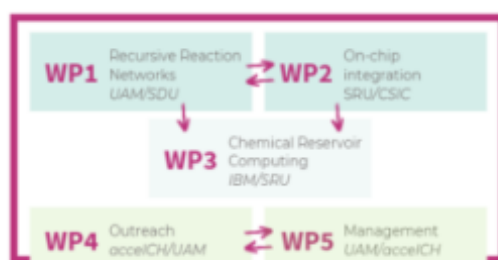
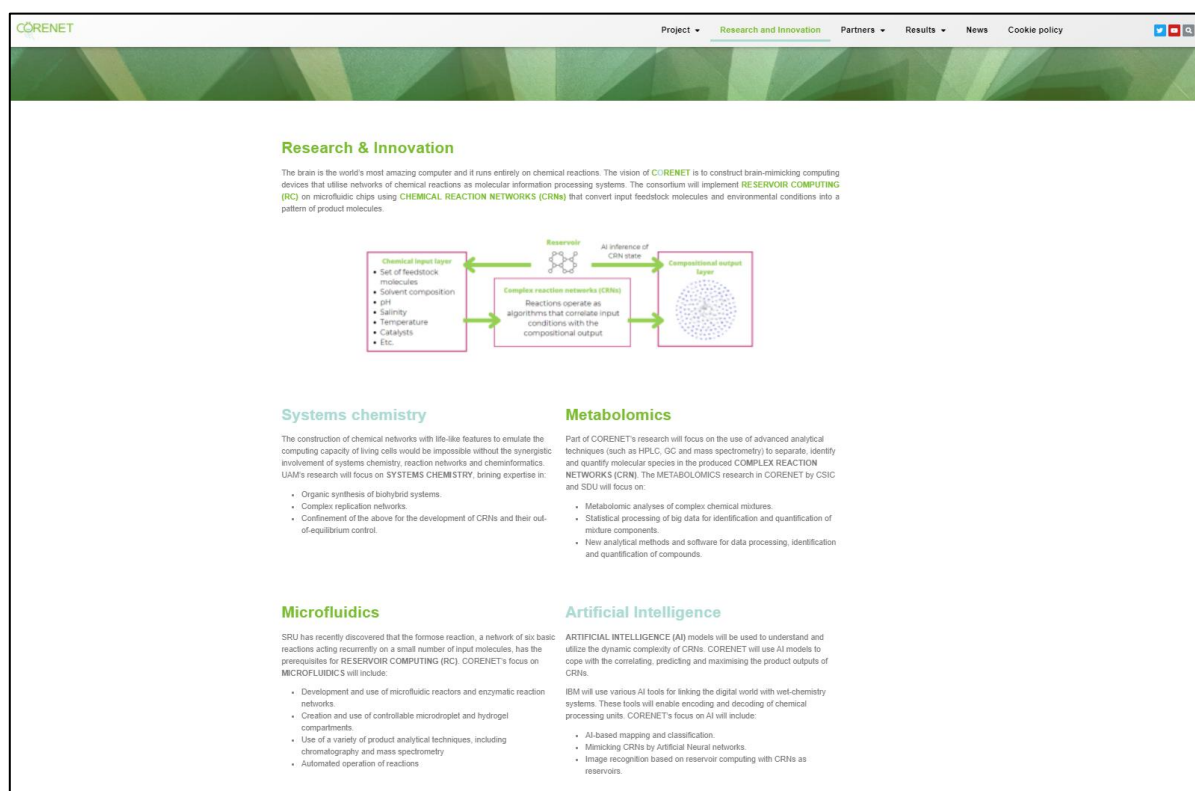


Figure 6: Overview of the 'CORENET's work plan' page accessible in the submenu of the key menu 'Home'

5.3 Research and innovation

The [Research & Innovation](#) page includes details on technological, innovative and application aspects of the CORENET project (see Figure 7). This page is mainly addressed to the research community (researchers in chemistry, artificial intelligence, computer science and the scientific community in general), industry and policymakers. This page will be enriched with visuals about data processing, AI models, digital platforms, among others throughout the project duration.



Research & Innovation

The brain is the world's most amazing computer and it runs entirely on chemical reactions. The vision of CORENET is to construct brain-mimicking computing devices that utilise networks of chemical reactions as molecular information processing systems. The consortium will implement RESERVOIR COMPUTING (RC) on microfluidic chips using CHEMICAL REACTION NETWORKS (CRNs) that convert input feedback molecules and environmental conditions into a pattern of product molecules.

Chemical input layer

- Set of feedback molecules
- Solvent composition
- pH
- Salinity
- Temperature
- Catalysts
- Etc.

Reservoir

Complex reaction networks (CRNs)

Reactions operate as algorithms that correlate input conditions with the compositional output

AI inference of CRN state

Compositional output layer

Systems chemistry

The construction of chemical networks with life-like features to emulate the computing capacity of living cells would be impossible without the synergistic involvement of systems chemistry, reaction networks and cheminformatics. UAM's research will focus on SYSTEMS CHEMISTRY, bringing expertise in:

- Organic synthesis of bihybrid systems.
- Complex replication networks.
- Confinement of the above for the development of CRNs and their out-of-equilibrium control.

Metabolomics

Part of CORENET's research will focus on the use of advanced analytical techniques (such as HPLC, GC and mass spectrometry) to separate, identify and quantify molecular species in the produced COMPLEX REACTION NETWORKS (CRN). The METABOLOMICS research in CORENET by CSIC and SDU will focus on:

- Metabolomic analyses of complex chemical mixtures.
- Statistical processing of big data for identification and quantification of mixture components.
- New analytical methods and software for data processing, identification and quantification of compounds.

Microfluidics

SRU has recently discovered that the formose reaction, a network of six basic reactions acting recurrently on a small number of input molecules, has the prerequisites for RESERVOIR COMPUTING (RC). CORENET's focus on MICROFLUIDICS will include:

- Development and use of microfluidic reactors and enzymatic reaction networks.
- Creation and use of controllable microdroplet and hydrogel compartments.
- Use of a variety of product analytical techniques, including chromatography and mass spectrometry.
- Automated operation of reactions.

Artificial Intelligence

ARTIFICIAL INTELLIGENCE (AI) models will be used to understand and utilize the dynamic complexity of CRNs. CORENET will use AI models to cope with the correlating, predicting and maximising the product outputs of CRNs.

IBM will use various AI tools for linking the digital world with wet-chemistry systems. These tools will enable encoding and decoding of chemical processing units. CORENET's focus on AI will include:

- AI-based mapping and classification.
- Mimicking CRNs by Artificial Neural networks.
- Image recognition based on reservoir computing with CRNs as reservoirs.

Figure 7: Overview of the 'Research and Innovation' page which is one of the key sections displayed on the Homepage

5.4 Partners

The [Partners](#) page provides details of the CORENET consortium with links to their respective websites, brief descriptions of each partner highlighting their expertise, as well as profile pictures and names of the team members involved in the project (see Figure 8). An interactive map represents the CORENET consortium in an attractive way that allows not only to zoom in and out but also to select individual partners from a list and see their exact locations. Links to the partners' websites are assigned to the site markers and redirect the user to the desired page in a new window.

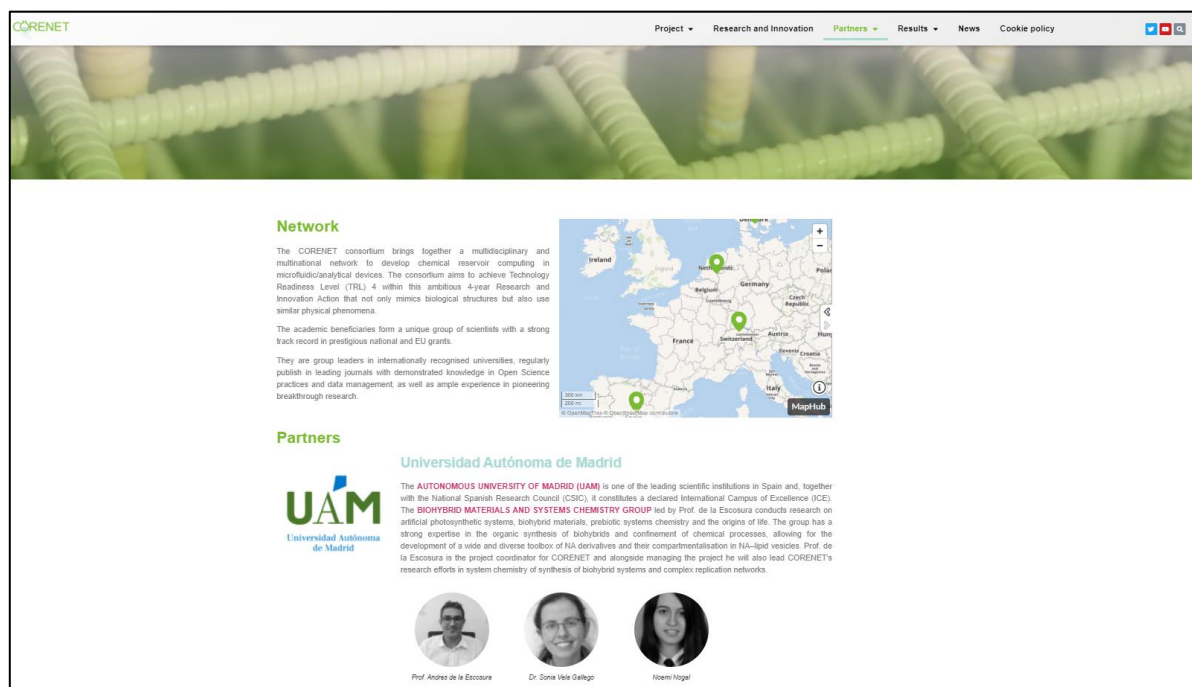


Figure 8: Overview of the 'Partners page' which is one of the key sections displayed on the Homepage

5.5 Results

This site provides stakeholders with the [latest achievements and publications](#) in the CORENET project. It includes at the moment a listing of background publications from CORENET researchers to understand the scope of the project from the very beginning. An updated list of the latest publications and publishable results of the CORENET research will be continuously integrated in the website.

5.6 News & events

The [News](#) page features short blog posts published whenever there is a worthy update regarding the project, or when news articles and any other related communication item of interest is released.

The page can be reached via the corresponding item in the main navigation menu or through the latest news items hyperlinked on the CORENET homepage. Each news piece is linked to its separate page, meaning that each post has an individual URL that can be shared.

5.7 Header and footer

The CORENET project increases its impact by being present on social media, namely Twitter and Youtube. Respective icons in both header and footer of every page give easy access to these digital platforms to all stakeholders (see Figure 9 and 10). To boost the outreach, information published on these channels is tailored not only to target audiences but is given in a way that aligns with the platform-specific requirements.

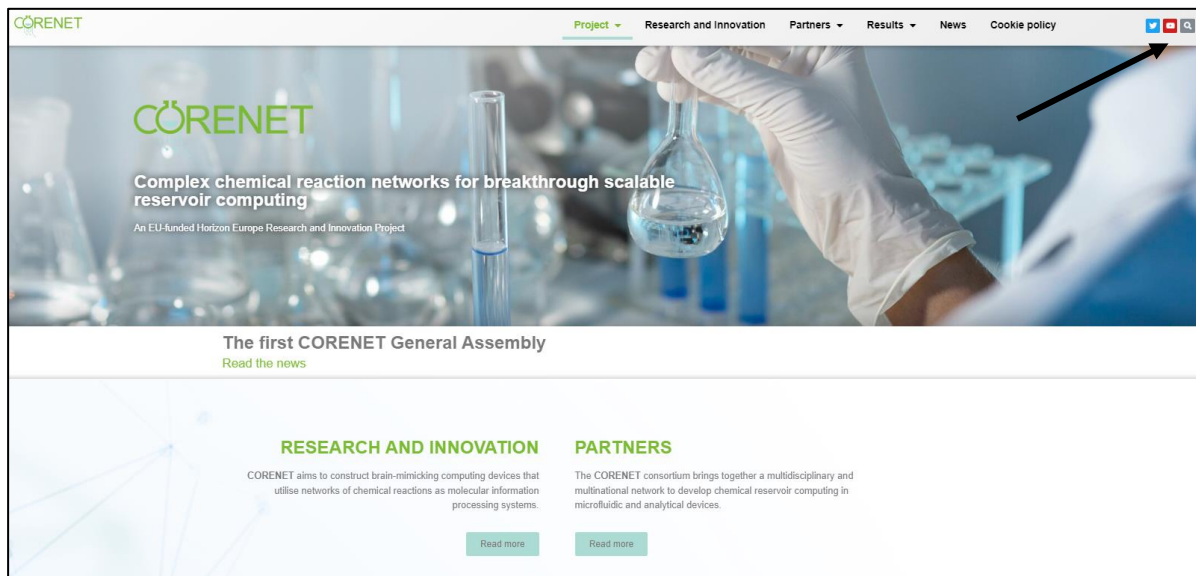


Figure 9: Overview of the social media icons on the CORENET website header

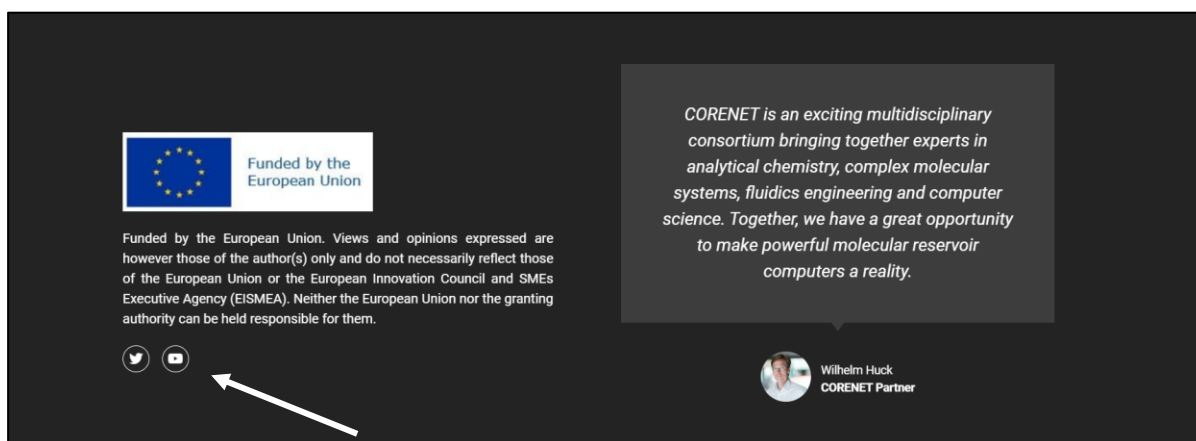


Figure 10: Overview of the social media icons on the CORENET website footer

6 Development & maintenance

The website will be continuously monitored and updated by accelCH, who will connect ideas and input from all CORENET partners and adjust accordingly. No information will be released without the previous approval of the consortium members.

The news and results sections are updated on a regular basis with upcoming events, news articles and achievements that are related to or of interest to the project and its stakeholders. Relevant documents and communication pieces will be made available to download on the CORENET website.

7 Outreach & evaluation

accelCH will measure the website's outreach with Google Analytics, which offers not only the possibility to track traffic (i.e., page views, clicks, and visitors), but can also detect the immediate impact of dissemination activities. These measurements will then be evaluated to ensure that the targets have been reached and to identify new outreach measures when necessary.

8 Outlook

The next steps in the development of the CORENET website will be to populate the news and results sites as achievements are reached and consortium meetings organised. Furthermore, the open positions site will be updated as new positions are created and fulfilled.

As the project progresses, a dedicated site will be created to accommodate the corresponding deliverables and results.

Overall, all pages will be updated with additional visual material as the project progresses, to ensure a visually pleasing, clear, and engaging experience for the website viewer. This includes embedded videos, photos from conferences, webinars and workshops, infographics, slideshows and other multimedia features that align with the CORENET visual identity.