

Making powerful molecular computers a reality — a prominent goal of the new Horizon Europe project CORENET

CORENET aims to implement reservoir computing based on reaction networks that can be used to sense and interact with living systems.

Chemists invest substantial time in repetitive experimental tasks, such as reaction monitoring and iterative optimisation. These activities limit the amount of time to other innovative and creative endeavours¹. Traditional chemical synthesis is a junction of the clever application of accumulated knowledge and art. The recent technological revolution with the development of robotics, microfluidics, integrated analytics and artificial intelligence (AI)-based data integration is leading to the programmable synthesis of molecules using computer-controlled devices^{2,3}.

This change of paradigm opens new opportunities to push chemistry beyond the synthesis of molecules to the synthesis of complex reaction networks (CRNs), which in living organisms control all essential processes⁴. CORENET's goal is to **construct chemical systems that can perform high-level computation based on chemical reactions**. *En route* to such a goal, **reservoir computing (RC)** is one approach that has shown high potential to overcome the limitations of traditional computing architectures with a low computational training effort.

Entering a new era of chemical science

The underlying idea of CORENET is to use the potential of CRNs to create a chemical RC system in which molecules are generated as a result of high-level computations performed by molecular ensembles left to freely react within a microfluidic device. The **implementation of material computing using chemical reactions has long been postulated but never realised**, mostly because the underlying chemistry needs to be executed in the most reproducible manner, which can only be achieved with the best-performing reactor hardware.

Understanding complex chemical systems is a major goal of current science, which will bring technological advances in chemistry and materials science. CORENET will face this grand challenge with an extraordinary group of academic and industry scientists working on systems chemistry, microfluidics, metabolomics and AI.

Andres de la Escosura, CORENET Coordinator

The main goal of CORENET is to **harness the potential of CRNs** to create powerful chemical reservoir computing systems. This molecule-based computing power enables truly sustainable AI, which speaks the language of living systems and can constantly process information about their molecular environment.

In such a way, CORENET will lay the foundations for a new era in the chemical sciences with scalable and energyefficient systems that can directly interface with living organisms.



Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Innovation Council and SMEs Executive Agency (EISMEA). Neither the European Union nor the granting authority can be held responsible for them.

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Achieving the goal through multidisciplinary cooperation

CORENET brings together 4 leading research groups with complementary expertise that covers all fundamental aspects of the project: <u>Universidad Autónoma de Madrid</u>, <u>Stichting Radboud Universiteit</u>, <u>Consejo Superior de</u> <u>Investigaciones Científicas</u> and <u>Syddansk Universitet</u>.

Their expertise is combined with the world-class knowledge in AI and machine learning modelling of a high-tech global industrial partner – <u>IBM Research Europe – Zurich</u>, providing in addition reactor hardware and <u>accelopment Schweiz</u> <u>AG</u> – specialised in project and innovation management and leading the communication and dissemination of the project. The activities in CORENET are divided into specific work packages (WPs), which are described in more detail on the project <u>Work Plan website</u> page.



CORENET team at the first General Assembly meeting, hosted by IBM Research Europe – Zurich, May 2022



CORENET Facts and Figures

CORENET is an EU-funded Horizon Europe Research and Innovation Project:

- Involves 6 partners from 4 countries
- Started on 1st of April 2022 and will end on the 31st of March 2026
- Budget: 3 million euro
- Website: corenet-horizon.eu
- Email: corenet.eu@gmail.com
- Coordinator Prof. Andrés de la Escosura, Universidad Autónoma de Madrid (UAM), Spain

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¹ Bédard, Anne-Catherine, Andrea Adamo, Kosi C. Aroh, M. Grace Russell, Aaron A. Bedermann, Jeremy Torosian, Brian Yue, Klavs F. Jensen, and Timothy F. Jamison. 'Reconfigurable System for Automated Optimization of Diverse Chemical Reactions'. *Science* 361, no. 6408 (21 September 2018): 1220–25. https://doi.org/10.1126/science.aat0650.

² a) Jamison et al., Science 2018, 361, 1220. b) Sach et al., Science 2018, 359, 429. c) Sanderson, Nature 2019, 568, 577.

³ a) Jensen et al., Science 2019, 365, 1-9. b) Grzybowski et al., Nature 2020, 558, 83. c) Seeberger et al., Angew. Chem. Int. Ed. 2021. d) Cronin et al., Nat. Chem. 2021, 13, 63.

⁴ Markvoort, Huck, de Greef et al., Chem. Soc. Rev. 2015, 44, 7465.