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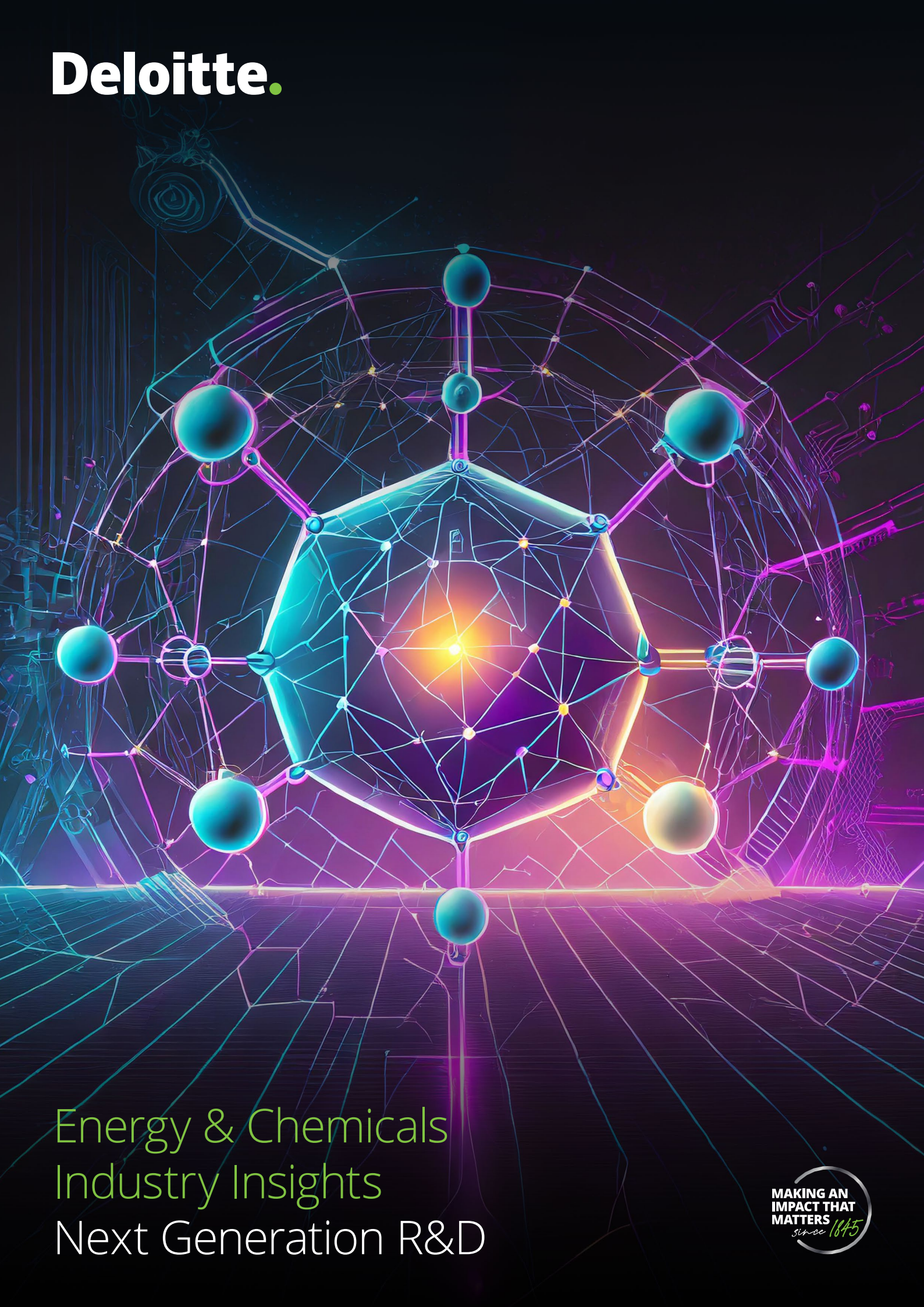

Energy & Chemicals Industry Insights

Next Generation R&D

MAKING AN IMPACT THAT MATTERS since 1845

The Next Generation of R&D

The future is here, but unevenly distributed.[1]

The future is already here, but its generative AI, quantum computing, cobots, avatar robots, data mesh and other technologies, new ways of working and complex ecosystems are not evenly distributed. Even the most innovative chemical companies must address the basics. Over 55% of data generated in research labs is unstructured or described as dark data – not used to derive any insights.[2] Over 50% of researchers struggle to repeat their experiments, and over 70% fail to replicate experiments done by others.[3] This in itself significantly reduces the innovative power of chemical and material science companies. Moreover, the new materials and solutions needed to power circularity, energy transition and a more sustainable economy require a new mindset, a new type of talent and new, elevated ecosystems.

To drive this future, innovation leaders in the chemical industry must ensure that their R&D is:

- Data- & tech-enabled
- Skill-based & talent-driven
- Alliance- & ecosystem-powered

Addressing all three aspects will provide the next generation of R&D at chemical and material science companies with the opportunity to deliver the solutions needed to power the future while offering a challenging and exciting environment for the next generation of innovators.

[1] William Gibson Quote and Deloitte "Tech Trends 2024", December 2023
[2] "Digital Transformation in the Chemical Industry: Steps to a Sustainable Future, J. Sexton, Chemical Abstract Services, Sept 2023
[3] "1,500 Scientists Lift the Lid on Reproducibility", M. Baker, Nature 533, 452-454 (2016)

The Forces Shaping Chemical Industry R&D

The next generation of R&D must turn unprecedented challenges into opportunity for the chemical industry

The chemical industry today faces unprecedented challenges, from geopolitical uncertainty and rapid energy transition to what many call “a regulatory tsunami.” Yet no other industry is better positioned for the necessary transformations, such as circularity, mobility, personalized health, energy transition... All of these require new and advanced materials and systems, delivered by chemical and material science companies in an ever shorter innovation cycle.

This dynamic world does not leave room for the old ways and mistakes of chemical company R&D departments. There is no room for “black data” or low reproducibility, and there is no room for the physical experiments and scale-ups done the “old way” either. The best experiment is the one not done at all - not on a lab bench nor in a scale-up facility. Instead, the best experiment is an in-silico experiment or a simulation suggested by an algorithm to narrow the experimental space as much as possible. The lab bench is reserved for a lucky few – a smaller number of selected, smart experiments that yield the most useful, reproducible data for rapid, data-based decision-making, probably done by machines, and only monitored or checked by researchers.

You will probably not find your next best idea in a lab, but rather in a complex ecosystem that follows the life cycle of a molecule or material from the cradle to the grave after several recycling lives. Your next best employee might not be a chemistry Ph.D. graduate but a skillful machine learning engineer hired from a deep tech start-up. And your next competitor might not be a chemical company but a smart tech one.

Future R&D must find the solution for all these challenges, and fast. The chemical industry lags behind in the digitalization and adoption of novel technologies. Chemical company R&D must change all four wheels while driving at full speed ahead to position itself for the future. This is a difficult transformation.

The R&D department of a chemical company must change its wheels while driving full speed ahead.

Three elements must be addressed simultaneously to ensure success:

- **Data- & tech-enabled R&D.** A new and uplifted R&D must emerge, one where a seamless merger of science and tech, physical and virtual worlds boost innovation and accelerate time to market. With the Scientific Internet of Things (SIoT), (Generative) AI and soon quantum computing, we are reaching a new age of data-driven decision-making in R&D departments at chemical and material science companies.

- **Skill-based & talent-driven R&D.** For true chemistry to happen, data- and tech-enabled R&D is only the first component. Next is the right combination of skills and talents to drive discovery and commercialization. Faced with the complex challenges of chemical companies, ever more complex emerging technologies, and the redefinition of work and workforce, R&D departments must look into the larger workforce ecosystem for the necessary skills and talents.

- **Alliance- & ecosystem-powered R&D.** The third ingredient requires stepping outside the box and joining or orchestrating larger ecosystems to drive purposeful innovation, growing the top line but also addressing significant economic and societal challenges. Collaboration and co-creation are essential to innovation in a complex environment.


AI generated

Chemistry meets Tech: Data- & Tech- Enabled R&D

Deep tech is opening new opportunities for R&D in the chemical and material science industries

At the core of the most pressing challenges of our era, including climate change, energy transition, accessible health care, food security, new mobility and many more, are chemistry and material science issues. These new challenges are so complex that the traditional approaches relying on experiment design and trial-and-error, researcher intuition and serendipity of innovation, are insufficient to find solutions. The next generation of R&D is needed. The one where seamless integration of chemistry and deep tech, real and virtual worlds, experiments and simulations lead to smarter innovation.

The next generation of R&D is fueled by (generative) artificial intelligence, quantum computing, high performance computing, data mesh, robotics, the metaverse, and the Scientific Internet of Things. Next generation R&D is more deeply tech-driven than ever before. It is no wonder that leading high-tech companies such as Microsoft, Amazon, and Google are competing for this space. At the time of writing, Sandbox AQ announced the acquisition of Good Chemistry to boost their AI simulation platform for drug discovery and material design.[1] Microsoft announced major activities with their Azure Quantum Elements platform to accelerate material discovery with AI and HPC. One of the first applications was screening over 32 million candidates to find better battery material.[2]

Amazon Web Services reported close work with the Lawrence Berkley National Laboratory on accelerating new material design.[3] And tech leaders such as IBM, Google, Amazon and start-ups in the quantum computing ecosystem are exploring the use of quantum computing in the chemical and material science industries.

These examples only illustrate the change that is happening within the R&D departments of chemical and material science companies. It is not about experimentation anymore. It is about smart experiments and improved molecular and reaction modeling, and simulations that will facilitate the discoveries needed to solve our current challenges.

The R&D laboratory landscape is undergoing profound change spurred by the cloud, 5G, and connected sensors and devices. The Scientific Internet of Things in the R&D labs brings the virtual and real worlds together to increase the scale and speed of chemicals and materials discovery.

Innovate smarter, not harder, using deep tech and Scientific IoT (SioT).

[1] "SandboxAQ Acquires Good Chemistry to Accelerate AI Simulation Platform for Drug Discovery and Material Science". SandboxAQ Company Announcement (2024) https://www.sandboxaq.com/press/sandboxaq-acquires-good-chemistry-to-accelerate-ai-simulation-platform-for-drug-discovery-and-material-science

[2] "Unlocking a New Era for Scientific Discovery with AI: How Microsoft's AI screened over 32 Million Candidates to Find a Better Battery". Microsoft Azure Quantum Blog (2024) https://cloudblogs.microsoft.com/quantum/2024/01/09/unlocking-a-new-era-for-scientific-discovery-with-ai-how-microsofts-ai-screened-over-32-million-candidates-to-find-a-better-battery/

[3] „Accelerating New Materials Design with Open Data on AWS". AWS Blog (2022) Accelerating new materials design with open data on AWS | AWS Public Sector Blog (amazon.com)

The era of serendipitous scientific discovery is over. It is time for smarter, scalable, and faster discoveries in the chemicals and material sciences. By embracing data-driven, technological advancements, the R&Ds of chemical and material science companies are set to uncover new frontiers, accelerate breakthroughs, and revolutionize the industry while solving the most challenging problems of our era.

The next generation of R&D is more data- and tech-driven than ever before. To succeed in this new reality, next generation R&D leaders must:

- Boost modeling and simulation capabilities
- Embed deep tech into R&D workflows
- Bring R&D cybersecurity up to date

Boosting modeling and simulation capabilities

Shorter innovation cycles and complex challenges have the cost of discovery skyrocketing. This gives in-silico experiments and simulations a new push. Different companies are at different maturity levels when it comes to molecular and reaction modeling and simulations. For years, the R&D departments of the leading chemical companies have translated chemical problems into computational models. The development of reliable mechanistic and statistical models required long-term strategic vision, considerable investment, highly skilled in-house talent, and often alliances with leading universities and research institutions, not to mention years of development. Very often these models were the result of decades of expensive, proprietary, in-house modeling development by highly skilled and experienced researchers. Companies that mastered modeling and simulations of a triangle between reaction conditions, molecular structure, and final product properties enjoyed a substantial payoff in terms of reduced development costs and accelerated time to market. They were also able to attract top talent from around the world for their R&D departments. Other chemical companies have not been able to make the investment in modeling and simulation capabilities and followed more traditional approaches in their discovery process.

Generative AI, cloud, high performance, and powerful universal quantum computers will soon bring next generation R&D modeling and simulations to the next level. Both leaders and followers thus have some homework to do. Anyone not yet fully utilizing the modeling and simulations in their R&D workflows must evaluate their current maturity level and make some strategic moves to digitalize their R&D workflows as soon as possible, and start building models based on historical data to increase their capabilities and set the stage for the future. The leaders, on the other hand, have already built their modeling and simulation capabilities. They need, or have already started, to experiment with the novel technologies, looking into various foundation models as a basis for different applications of (gen)AI in R&D. They are also exploring quantum machine learning in itself or in combination with AI to boost their simulation and modeling capabilities. Not to mention the range of companies acquiring and/or upgrading their high-performance computers for more computing power to drive complex molecular modeling, in-silico experiments and simulations.

Embedding deep tech into R&D workflows

A number of new technologies are promising to reshape the state-of-the-art R&D departments of chemical and material science companies. The new technologies are opening new avenues for R&D at any stage of industrial discovery, including the digitalization of the ideation phase by using AI and content analytics to screen various internal and external sources, using open innovation and co-creation platforms to get new ideas for using AI, and soon quantum computing for modeling and simulating to narrow the experimental space for the next best experiment. Once in the lab, the Scientific Internet of Things offers a real-time connection between physical lab sensors and IoT devices, enabling real-time data collection and analysis, as well as suggestions for corrective actions and the next best steps.

Combining emerging technologies such as Gen (AI) and quantum computing with existing high-performance computing will considerably accelerate material discovery.

Here are just some of the technologies R&D leaders should be exploring:

Data mesh is an architectural paradigm that focuses on decentralizing data ownership and management in large organizations. It aims to give cross-functional teams direct access to the data they need for their specific use cases while maintaining data quality, governance, and security. Data mesh can revolutionize chemicals research by democratizing data access, promoting collaboration, enhancing data quality, and empowering researchers to leverage data in innovative ways. It aligns with the industry's increasing reliance on data-driven insight and positions chemicals research for continued progress and growth.

(Generative) Artificial intelligence has the power to augment human capability in research laboratories. AI algorithms can integrate data from multiple sources, analyze vast amounts of data, identify patterns, and generate valuable insights. It can assist researchers in designing experiments, predicting chemical reactions, and accelerating the discovery of new materials. Some estimates predict a Generative AI share in the chemicals market of $1.2 bn by 2030, but only for AI models that generate new components and predict their properties.[4] AI can also optimize laboratory workflows, automating routine tasks and freeing up scientists' time for more complex and creative endeavors. AI can integrate data from different stages of the innovation process, screen internal and external data sources, and conduct simulations, experimentation, and quality control for easier and faster data-based decision-making. R&D labs can leverage machine learning and AI algorithms to identify patterns and anomalies in data, predict potential issues, and optimize experimental processes for improved data quality. The day is not far when a reinforcement learning-based AI algorithm might ensure autonomous control of complex laboratories and run the labs without human intervention. Especially interesting is the autonomous control of high-throughput labs using AI, where not only execution but data analysis and data-based decision-making is done without human intervention.

Quantum computing offers immense computational power and the possibility to simulate complex problems in a way that is not possible using classical computers. Today, identifying a solution among a vast number of possibilities is based on assumption and simplification to such an extent that we might not have a true solution at all but rather some local optimum. This will change with the use of quantum, enabling new insights into complex systems with a vast number of variables using quantum mechanical principles. The chemical industry will be among the first to benefit from quantum computing, once quantum computers have enough power to address complex problems. We will be one giant step closer to modeling and simulating a "holy grail" of chemistry - the structure-property relation of complex materials.[5] Quantum simulations will offer insight into chemical reaction mechanisms for more precise selection of reactants and reaction conditions. This will provide completely new insights into the design of the materials we need for a better future, like improved batteries, highly selective active ingredients for medicine and crop-protection, and efficient organic metal frameworks for carbon capture, to name a few. Although experts and futurists do not agree on when exactly we will have a fully functional universal quantum computer, all agree that to win the quantum race they must start experimenting with quantum now. Some strategic simulations indicate that those not preparing for quantum computing now will not be able to compete with companies already exploring quantum. The impact of quantum computing will be much faster and more forceful than the impact of (Gen) AI. Moreover, the lack of a quantum-literate workforce will be a limiting factor. To maximize the benefit of quantum computing, R&D leaders must start now to identify relevant quantum use cases, ensure access to a quantum workforce either internally or as part of their workforce ecosystem and finally, work on overall quantum computing strategy.[5]

Transitioning from monolithic data warehouses and data lake monsters toward a distributed data mesh allows R&D teams to unlock the full potential of their data

[4] Generative AI in Chemical Market: Current Analysis and Forecast (2023-2030). Report UMTI212276. UnivDatos Market Insights. https://univdatos.com/report/generative-ai-in-chemical-market/

[5] „Quantum computing isn't hype it's ushering in a new era". R. Jovanovic, Handelsblatt (24.Jan.2023) https://www.handelsblatt.com/meinung/gastbeitraege/gastkommentar-quanten-computing-ist-kein-hype-sondern-leitet-eine-neue-aera-ein/28928958.html

The Scientific Internet of Things (SIoT) connects devices and sensors, enabling real-time data collection and analysis in research laboratories. IoT devices can monitor experiments, capture environmental variables, and ensure optimal conditions for chemical processes. The integration of IoT into research labs facilitates remote monitoring, enhances data accuracy, and supports predictive maintenance, enabling proactive decision-making and efficient resource management. This includes the use of high-throughput screening and combinatorial chemistry approaches to enable labs to rapidly test large numbers of compounds and optimize chemical processes. To fully benefit from the SIoT, R&D leaders must ensure that the digitalization of lab processes in particular does not stall.

Robotics technology is revolutionizing research laboratories, enabling automation, precision, and reproducibility. Robotic arms can perform repetitive tasks with high accuracy, reducing human error and enhancing experimental consistency. Automated sample handling, compound synthesis, and high-throughput screening contribute to faster research cycles and accelerated innovation. Robotics is a basis for mobile laboratory operations as well as for remote-controlled laboratories. It enhances safety by handling hazardous substances and performing experiments in controlled environments. With the recent advances in robotics, AI, and Scientific IoT we might be closer to fully automated, "lights out" laboratories soon.

The industrial metaverse positively impacts R&D labs in the chemicals industry through virtual experimentation, collaborative innovation, data-driven decision-making, and real-time visualization. It enhances operative work by enabling scientists to conduct complex experiments virtually, fostering global collaboration, and providing valuable insights for optimized outcomes. With immersive visualization and skill development opportunities, the metaverse empowers researchers to drive groundbreaking discoveries and increased efficiency.

Bringing R&D cybersecurity up to date

The security perimeter is no more. Cloud solutions, generative AI, quantum computing, edge applications, SIoT, IT/OT integration, mobile apps, and other digital innovations —they all blur the boundaries of today's R&D environment. While driving research forward, these technologies also pose big questions about how to secure modern research, especially when skilled resources are scarce and architectures ever more complex.

Organizations must face this new reality in which there no longer exists a perimeter to protect, and the use of legacy tools and tactics can be ineffective, unreliable, and difficult to support. They face modern security needs but rely on antiquated security architecture that does not respond to today's environment, framed by challenges and opportunities.

Zero Trust allows organizations to operate on the principles of least-privileged access and context-aware authentication, with a "never trust, always verify" approach to providing globally distributed R&D teams access to data, systems, services, and other resources. Its modern approach securely connects users and devices to applications over any network that complies with policies and contextual data, instead of automatically granting access based on network location. Nevertheless, trust in many ways is a mindset shift—less about making the network comply with policy, and more about establishing context for a connection request before granting access.

The scientific IoT is a seamless integration of real-time data from sensor-equipped lab devices, data generated by in-silico simulations, external data, and experimental data, resulting in streamlined workflows, enhanced reproducibility, and acceleration of material discovery

The chemical industry is not an early adopter of new technology. Despite the promises of data-driven R&D, several challenges impede the seamless integration of data-driven technologies within the chemicals industry. Identifying and addressing these blockers is vital to creating a roadmap towards a future where data-driven R&D becomes the norm. R&D leaders must find the path to overcome these challenges:

1. Heterogeneity of Data
R&D accumulates vast amounts of data from various sources, such as experiments, simulations, and external databases. The diverse formats, structures, and quality of this data make it challenging to consolidate and extract meaningful insights.

2. Incremental Innovation
Tradition and risk-aversion can limit the willingness to adopt transformative technologies. In some cases, a preference for incremental innovation over disruptive change hinders the full integration of data-driven methodologies.

3. Localized and Little Coordination
In large organizations, R&D efforts are often dispersed across different teams, sites, and countries. This decentralized approach, while beneficial for innovation linked to local markets, can hinder collaboration and information sharing, leading to missed opportunities. A healthy balance between centralized and decentralized activity is required.

4. Mode of Work and Processes
Legacy workflows and practices may not align with the demands of data-driven R&D. Adapting to new ways of working and adopting agile, data-centric processes can be challenging but crucial. Rather than just embedding new technologies into existing R&D processes, R&D leaders must use the emergence of new technologies to completely re-design R&D processes.

5. Lack of Data Visualization
Converting complex data into visually intuitive representations is a vital aspect of data-driven decision-making. The absence of effective data visualization tools can limit the understanding and communication of critical insights.

Getting your R&D data-driven and tech-enabled takes more than just implementing the newest LIMIS software or upgrading outdated hardware. It requires a holistic transformation that reshapes how researchers approach the challenge, decide on the next best experiment, capture their own and learn from existing knowledge, and collaborate internally and externally

Summary

Next generation R&D must solve some of the biggest challenges of our time to ensure sustainability, future mobility, and to enable access to better food and medicine for billions of people on the planet at a time when the chemical industry is facing unprecedented challenges. There is no longer room for serendipity in chemical and material science discovery.

It is time to innovate smarter, not harder, using the advantages of emerging technologies such as (generative) AI, the Scientific IoT, robotics, and soon quantum computing and the metaverse. R&D departments will become more efficient, productive, and innovative. Simultaneously, R&D leaders must address the most common obstacles, such as heterogeneity of R&D data, risk aversion, isolation of R&D, legacy workflows and practices, and the lack of data visualization.

There are three priorities for R&D leaders to fully benefit from data- and tech-driven R&D:

- Boost modeling and simulation capabilities
- Embed deep tech into R&D workflows
- Bring R&D cybersecurity up to date

With shorter and shorter innovation cycles, modeling and simulation capabilities are the true competitive advantage of a chemical company. Boosting these capabilities is a must for chemical and material science leaders to solve complex future challenges.

Embedding deep-tech into R&D workflows at any discovery stage will increase the innovative power of next generation R&D. It's all about merging the real and the virtual worlds for smarter, faster, and scalable discovery.

R&D leaders also need to bring R&D cybersecurity up to date. It is not only about preventing cyber attacks on the most critical infrastructure; it is also about enabling a safe and secure collaboration within larger and more complex ecosystems.


AI generated

Focusing on people: Skill-based and Talent-Driven R&D

People are the main drivers of the success and sustainability of future R&D – beyond all technology and innovation.

When we talk about ever-growing challenges, emerging technologies, and the digital revolution within the chemicals industry, we must keep in mind that ultimately it is all about people. The people within the chemical companies who find innovative solutions every day and keep the market running. They are the heart of the change the chemical industry is currently undergoing.

The future of R&D involves disruptive products solving our biggest economic and societal challenges by using cutting-edge technologies – but that's only half the truth. Because in the end, no matter how groundbreaking future R&D is, if not designed with people in mind, the company will not reap its full benefits. It is the people who drive innovation, bring products to life, ensure quality, and foster customer experience. Their expertise, creativity and adaptability are crucial to the success and sustainability of the chemicals industry, especially in a rapidly changing world.

But how to get your R&D workforce future-ready? And how to ensure that you bring the people along on your transformation journey towards the R&D of the future?

Below are three key activities to help you set the scene for your future skill-based and talent-driven R&D. We shed light on why the R&D workforce needs to be more diverse than ever before, why future-proof skills matter, why new ways of working need to be embraced, and why a harmonious blend of R&D employees and cutting-edge technologies is inevitable.

- Focusing on skills and diversify your teams
- Stepping into a new reality: Merging the physical & digital worlds
- Embracing new ways of working

The future of R&D will require boundaryless collaboration within larger ecosystems enabled by technology.

Focusing on skills and diversity in R&D teams

What if we told you that the traditional roles in companies and in R&D are outdated? What does that mean? Deloitte's 2023 Global Human Capital Trends[1] clearly shows skills as the primary focus for matching workers and work. Skills are already replacing strict roles, a legacy from the industrial age. In the future, it will be less about specific job titles, formal definitions or degrees, and more about the ability to work across set job boundaries within much larger and more complex ecosystems. This shift is critical for chemical companies to remain competent, respond flexibly to change, and address talent shortages. Over 60% of R&D leadership reports difficulties in filling R&D openings, according to a recent Gartner study.[2]

It is not surprising that the increasing digitalization of the R&D environment and processes is changing the skills and capabilities within R&D. The chemical industry increasingly relies on various digital skills to drive innovation, efficiency, and competitiveness as new technologies emerge. Data analytics, machine learning, quantum computing, the Scientific Internet of Things (SIoT), robotics and automation are no longer buzzwords but R&D reality. Advanced soft skills such as problem solving, critical thinking, and creativity play an ever more important role in a world where real and synthetic data merge beyond recognition, and making sense of it all might be the most important skill of them all.

Companies must ask themselves, "What needs to be done?" and "Which skills are required?". It is not solely about focusing on tech skills such as machine learning, AI or quantum computing but rather a merging of these capabilities with a strong foundation in domain-specific knowledge, including chemistry, materials science, and chemical engineering. These are all in-demand, hard-to-find skills. R&D leaders must cast a wider look at the workforce ecosystem to fill the openings e.g., free-lancers, digital nomads, and retired employees with the knowledge and experience.[1,3] Furthermore, and due to the complexity of the problems the chemical industry is trying to solve, future R&D work models might involve an on-demand workforce that works simultaneously for several chemical companies, even in a sensitive environment such as R&D. Models that "share" employees with partners in an ecosystem are also possible. These models will require a new type of R&D leadership capable of orchestrating such workforce ecosystems, guiding employees with a different understanding of and relationship to work, all while gaining competitive advantage in such a complex environment.

Do I need to change my entire workforce to meet these requirements? The clear answer is no. Companies must identify current skills gaps and provide tailored learning

[1] "2023 Global Human Capital Trends". Deloitte Report (2023) https://www2.deloitte.com/us/en/insights/focus/human-capital-trends.html?icid=learn_more_content_click
[2] "Leadership Vision for 2024: Top 3 Strategic Priorities for R&D Leaders". Gartner Report (2023)
[3] "Do You Need an External Talent Cloud". J. Winsor and J.H. Paik, Harvard Business Review (Jan 2024)

journeys. This should be done using innovative approaches and digital tools such as the Metaverse, great for creating a unique learning experience by replicating real-world lab environments. Learners can conduct virtual experiments, operate equipment virtually, and analyze data in a realistic digital environment. Re-skilling and upskilling STEM professionals usually employed in R&D is one of the routes available to R&D leaders for addressing the skills shortage. For example, the US government has developed strategic plans to upskill STEM professionals into the QSTEM (Quantum STEM) to address the shortage of quantum computing skills, which will only become more acute.[4]

In addition to re-skilling, upskilling and continuous learning, a proper employer brand and talent marketing strategy should be pursued to attract new talent, especially digital natives, and to break the traditional perception of R&D labs and R&D career stereotypes. Chemical companies not only compete with other chemical companies for talent, but must also compete with the tech giants whose brands are much more attractive to digital natives, as well as to start-ups and their enticing purpose-led missions. It has never been more important for chemical companies and especially their R&D departments to exploit the brand and have a clear talent marketing strategy.

Diversifying skills and teams to increase competitiveness by taking a more holistic approach to the R&D workforce creates a workforce ecosystem that reaches beyond R&D and corporate boundaries.

Stepping into a new reality where the physical and virtual worlds merge

New technologies emerge every day and rapidly enter the R&D workplace where, despite being mostly early adopters, there is still a fear of being replaced by technology. With each technological advance, this fear intensifies and affects more and more people. We all may be wondering: will new technologies take over chemical labs and make scientists obsolete in the future?

It is actually more a question of learning to play together, since the traditional view of technology as a substitute for human labor is too narrow. Technology contributes to making work better for humans and humans better at work. In the context of R&D, this means that new technologies are not meant to replace R&D employees but to assist them in simplifying their work and fostering their creativity. But how can emerging technologies such as cobots and GenAI become real "discovery partners"? And how can we establish a symbiotic relationship between human and technology?

Some R&D employees spend hours in laboratories, repeatedly conducting the same experiment and carrying out the same meticulous preparation and tasks. Integrating new technologies such as cobots

[4] "Quantum Information Science and Technology Workforce Development National Strategic Plan". The USA National Science & Technology Council Report (2022). https://www.quantum.gov/wp-content/uploads/2022/02/QIST-Natl-Workforce-Plan.pdf

into these labs would free employees from these repetitive tasks. Work and daily life in the laboratory is completely transformed. By "cutting out the middleman", or rather the “middle tasks”, R&D employees are free to devote themselves to the innovative part of their work, without distraction, and to let their creativity and curiosity shine. Lab sensors, devices and instruments connected to the Scientific Internet of Things monitored and controlled by AI systems, harvest enormous amounts of data, enabling data-driven decision-making in R&D as never before, and enabling R&D employees to make even the toughest decisions with more confidence and speed for accelerated time to market.

A new field of experimentation and expression is opening to scientists, who shouldn't be afraid of being replaced by new technologies but rather embrace the new possibilities offered to enrich their work experience and support their decision-making.

To enable this new human to machine collaboration, companies must explore and invest in the new technologies. A period of adaptation will allow employees to familiarize themselves with the new tools, and a proper adaptation and engagement journey will set the scene for the future.

Embracing new ways of working

The chemical industry is highly competitive, and companies are constantly looking for new products and processes to stay ahead. With rapidly changing customer demands and market dynamics, the "how" of doing things will hold more significance in the future. How can companies accelerate innovation? How can they foster knowledge exchange and build up knowledge? And how can they effectively tackle complex challenges? New ways of working can help companies raise their R&D game to the next level and ultimately enhance productivity as well as efficiency.

The COVID-19 pandemic has changed our lives and the way we work, moving from on-site to remote working spaces. Surprisingly, this change was smoother than many companies expected, and in the chemicals industry as well. So why wouldn't it work out for R&D Labs in the long run? The answer is it can and should. As the workforce changes and the demands of new generations drive this change, R&D must prioritize remote work opportunities, flexibility, and even shorten the work week to stay attractive for different types of talent.

R&D in the chemical industry is adopting software industry practices like agile ways of working and rapid prototyping. It is setting the stage for the new ways of working required for ever shorter innovation cycles, where rapid prototyping and closer B2B-customer and end-customer feedback is an integral part of product design. Using genAI capabilities to “scrape” accumulated knowledge from the past and embed it into product design from day one using genAI assistants is quickly becoming reality in R&D.

The boundaryless collaboration required to innovate in complex ecosystems is a new way of working that requires an open mindset, data transparency, and the ability to work in conventional as well as virtual "cloud labs". Enabled by cutting-edge technology, virtual labs leverage data, the Scientific IoT and cloud-based infrastructure to facilitate seamless, real-time collaboration across companies and geographic boundaries. Multiple researchers from different companies within a given ecosystem can, for instance, work simultaneously on the same project, promoting efficient teamwork and reducing the need for physical presence at the same location.

This type of collaboration is not typical, unlike the individual alliances and less complex alliance portfolios we are used to in the chemical industry. They are massive and complex ecosystems that work with many companies, industries, regulators, government institutions and even NGOs and climate activists to solve challenges like closed loop recycling. This is a true test for the new way of working and collaboration readiness of individual stakeholders in such an ecosystem.

New ways of working pursue the faster scientific progress and innovation needed to solve enormous challenges, such as building a circular economy while staying competitive and harnessing the power of the workforce ecosystem while enabling and respecting the individuality of each R&D employee.

Summary

As the nature of work evolves and traditional jobs become increasingly fluid, focusing on skills allows R&D labs to adapt and thrive. By shifting away from strict roles, skill-based approaches enable employees to develop expertise and contribute to a range of responsibilities, fostering personal growth and job satisfaction.

Innovative approaches and digital tools optimize their learning experience, enabling employees to upskill and reskill efficiently and effectively. By showcasing a commitment to skills-based hiring and highlighting diversity and inclusion initiatives, R&D labs can differentiate themselves as desirable workplaces, attracting and retaining a diverse workforce that enhances overall performance.

While access to new technologies lays the foundation, it is the implementation and usage by lab personnel that truly makes a difference. Establishing a symbiotic relationship between technology and humans allows for seamless integration of these tools into daily lab practices, ultimately easing the scientist's work. It is essential for labs to quickly embrace these technologies, harnessing momentum and ensuring that employees are well prepared to use them effectively. The journey towards people-centricity should include employees initiating change, communication, and training measures from the very start. This emphasis on people will drive innovation and enable scientists to push the boundaries of scientific research.

Embracing new ways of working within R&D labs is essential to increasing innovation and enabling faster time to market. Flexible working and collaboration models which engage talent from a wider workforce ecosystem supported by enabling technologies like cloud-based infrastructure and deep tech are must-have rather than nice-to-have. The impact of new ways of working extends beyond R&D departments and enterprise boundaries, essential for solving complex challenges such as circularity, energy transition, and the journey toward the net zero economy.


AI generated

Where Ally Trumps Make and Buy: Alliance- and Ecosystem-Powered R&D

Next generation R&D is all about innovation and co-creation in complex, decentralized ecosystems that solve complex challenges.

Chemical companies have been balancing Make, buy, and ally for years[1]. Engaging with academics, research institutions, start-ups, customers, and suppliers has driven chemical and material science company innovation. Many managed their alliance portfolios and networks (more or less) systematically to increase innovation. The ROI on alliances has established itself as one of the KPIs for measuring the success of R&D investment.

Today, however, the bar for collaboration and co-creation is higher than ever. The complex challenges R&D departments are trying to solve require more and more complex, decentralized ecosystems rather than management of individual alliances, crowdsourcing competition or the occasional innovation hackathon. Only the strongest brands in the chemical industry will be able to set up such ecosystems. Others will primarily form part of the ecosystem value proposition and try to monetize their participation as much as possible.

The next generation of R&D is powered by alliances and ecosystems more than ever before. To succeed in this new reality, next generation R&D leaders must:

- Start thinking in ecosystems
- Get R&D data ready for data ecosystems
- Explore R&D's role in the monetization of ecosystems

Only the strongest brands will be able to design new and complex business ecosystems. Others will form part of the value proposition.

[1] "Balancing Make, Buy and Ally", R. Jovanovic and F. Broetzman, Performance, Volume 9, Issue 1, (2017)

Start thinking in ecosystems

Easier said than done. Especially since the definition of a business ecosystem is fluid and often combined with an orchestrated alliance network. True ecosystems are decentralized networks where each actor contributes to the overall value proposition while simultaneously getting their return on investment. If a single actor has the final say on who is joining and under which condition, this company is the orchestrator of an alliance network and not an ecosystem, no matter how complex the network is. True ecosystems operate as decentralized networks.

How to start thinking in ecosystems?

It starts with formulating the challenge you would like to solve (e.g., improved batteries, increased recyclability of commodity plastics) and identifying all actors and stakeholders involved in the solution. How are they connected today? What value proposition would get them to join forces? What is your role? Is your company's brand strong enough to orchestrate such a network, or are you joining as a contributor to an existing network or ecosystem? Brand power is one of the most important and complicated questions. Only a handful of chemical companies have a powerful brand and the presence to orchestrate complex alliance networks or serve as a catalyst for a true ecosystem. What's more, the competition is fierce, so even if you have a strong brand but are late to the table, you might not be able to grow a strong alliance network or ecosystem, so joining an existing network or ecosystem is more beneficial.

A fundamental requirement for ecosystem thinking is the right mindset. Change takes time. Fostering a growth mindset is a prerequisite for success. If your R&D strategy was oriented toward make and buy in the past, it will require effort to change overall R&D and company culture to consider alliances as a source of competitive advantage. This will take time and perhaps hiring different types of R&D talent who are more open to collaboration and co-creation with externals.

Getting R&D data ready for data ecosystems

R&D data ecosystems will be a prerequisite for the innovation of the future. There are several aspects to consider. Even if you are joining an ecosystem, you will be required to share R&D data with partners who may be close competitors. If your aim is to orchestrate complex innovation networks, your R&D data readiness is even more critical.

R&D data ecosystems accelerate innovation. You may not even know what kind of innovation will happen within such an ecosystem, but giving different actors the opportunity to access and explore data, collaborate and co-create within the ecosystem might lead to innovation. With the rise of AI, large language models based on data from various sources in a R&D data ecosystem will attract interest and lead to unprecedented competitive advantages for all actors involved.

To activate ecosystem thinking, it is essential to look beyond the R&D department and company borders when designing your R&D data strategy and architecture.

A starting point is to follow the FAIR guiding principles for scientific data management and stewardship published in 2016[2]. They apply to data, metadata and infrastructure. Here is a summary:

Findable. Data and metadata should be easy to find, preferably for both humans and machines.

Accessible. Users must know how to access data using authentication and authorization.

Interoperable. Data needs to interoperate with different applications and systems.

Reusable. Metadata and data should be well described so that they can be replicated and combined with other data.

Adhering to FAIR data principles will prepare R&D data for exchange with partners. Building an R&D data ecosystem will require much more from the decentralized setup of a business ecosystem. There is no single recipe for success here. However, the best data ecosystems are built around a platform that keeps the ecosystem together and enables its partners to integrate different data sources so that machine learning and analytics tools can collect, store, analyze, and play with the data.

Exploring R&D's role in the monetization of ecosystems

The chemical industry is essential to meeting global sustainability and circularity goals. Meeting these goals will require material and technological innovation from chemical companies alone or more likely from chemical companies in close collaboration with other actors within complex ecosystems.

For example, the rigid polyurethane (PU) foam used in the insulation of refrigerators. The recycling of rigid PU foam requires a complex ecosystem. The Circular Foam (circular-foam.eu) consortium comprises over 25 companies, universities, and research institutions from Germany, the Netherlands, Poland, Austria, Belgium and others. The European Union funds the project with almost 20 million euros.

The chemical recycling of rigid PU foam is one step among many in this closed material loop. But considerable R&D effort is required to develop and master chemical recycling. And it doesn't just involve chemistry, but a combination of atoms and bytes, a physical and virtual world. AI can be used to identify different materials, for instance, and prepare effective recycling or to predict the right feed of virgin and secondary raw material during processing to obtain the desired properties of the recycled material. There are so many possibilities for future R&D.

This is just one example of how the R&D of a chemical company can contribute to finding the right solution and help it monetize circularity. There are many to come.

[2] "The FAIR Guiding Principles for Scientific Data Management and Stewardship", M.D. Wilkinson et al., Scientific Data 3, 160018 (2016)

Summary

While chemical companies in the past were good at balancing Make, buy and ally to increase innovation, the collaboration bar has been set even higher. It is not enough to manage an alliance portfolio, have an open innovation platform or an occasional innovation hackathon. R&D departments must prepare to collaborate and co-create in complex ecosystems.

The next generation of R&D is powered by alliances and ecosystems more than ever before. To succeed in this new reality, next generation R&D leaders must:

- Start thinking in ecosystems
- Get R&D data ready for data ecosystems.
- Explore R&D's role in the monetization of ecosystems

The challenge faced, brand value, and mindset are aspects of ecosystems. The most dramatic cases might require a change in overall company culture to benefit from ecosystem thinking.

FAIR data is a good starting point for getting R&D data ready for ecosystems. But setting up and growing an R&D data system requires much more, there is no single recipe for success.

R&D plays a vital role in the monetization of ecosystems. It is is a combination of chemistry and technology, atoms and bytes, the physical and virtual for solving the complex challenges posed by sustainability and circularity goals.


AI generated

Conclusions

Increasing economic, geopolitical and regulatory uncertainty exposes today's chemical companies to unprecedented threats. At the same time, there are unprecedented opportunities for chemical and material science companies to become game changers by providing new generations of smart materials and solutions to address our most pressing challenges, such as reversing climate change, providing food and medicine for our growing population, and supporting new mobility solutions and energy transition.

In this highly dynamic environment requiring extraordinary collaborative and co-creative effort, there is no room for the "old" ways of innovation. There is no room for "black data," low reproducibility of experiments, or even for physical experimenting to the extent we have known in the past. The next best experiments are in-silico or simulated solutions suggested by an algorithm. The lab bench is reserved for a lucky few smart experiments. The lab is driven by the Scientific Internet of Things, which collects and analyzes data. Algorithms, monitored and supervised by researchers, decide the next best step. This is, in essence, the next generation of R&D.

Given that the chemical industry could more quickly digitalize and adopt new technologies, the R&D of chemical companies must undergo considerable change to reach the next level, analogous to changing all four wheels while driving at full speed.

To scale innovation and accelerate time to market, R&D leaders must ensure that their R&D is:

Data- and Tech-Enabled. Data- and tech-enabled R&D uses in-silico experiments, simulation, and modeling for competitive advantage. It has deep tech embedded in the R&D workflows to merge the real and virtual worlds for smarter, faster, and scalable discovery.

The Scientific Internet of Things is the critical enabler for the next generation of R&D labs. Cyber security's role is to protect R&D data and IP and prepare R&D to collaborate and co-create successfully in complex environments.

Skill-based and Talent-Driven. In a world where traditional roles and working models cease to exist, the next generation of R&D focuses on skills and workforce diversification to attract the broader talent needed for future success. R&D leaders must think in terms of workforce ecosystems to ensure the right skills and talents. In a new world where the real and virtual worlds merge, the latest technologies simplify work and foster creativity in unexpected ways. Embracing new ways of working is a prerequisite for attracting talent.

Alliance and Ecosystem Powered. Next generation R&D can only address challenges in a collaborative and co-creative environment. The rise of ecosystems is pushing chemical companies out of their comfort zones. Only the strongest brands, however, will be able to design new ecosystems. Others will be actors and part of the ecosystem value proposition. R&D leaders must start thinking in ecosystems instead of linear processes. They must prepare R&D data for use in data ecosystems and explore the role of R&D in monetizing ecosystems.

When all three aspects are developed continuously, the next generation of R&D will deliver solutions needed to power the future while offering an exciting environment for the next generation of innovators. One thing is certain – there has never been a better time to be a researcher at a chemical or material science company.

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