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Global AI-driven Materials R&D Software Market 2026 by Company, Regions, Type and Application, Forecast to 2032

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Abstracts

According to our (Global Info Research) latest study, the global AI-driven Materials R&D Software market size was valued at US$ 257 million in 2025 and is forecast to a readjusted size of US$ 878 million by 2032 with a CAGR of 19.0% during review period.

AI-driven Materials R&D Software refers to specialized software platforms that deeply integrate artificial intelligence technologies with materials science knowledge systems. The core attribute of this software lies in the use of machine learning, deep learning, generative models, and AI agents to digitally reconstruct and significantly accelerate traditional trial-and-error processes in materials research and development, including experimental screening, formulation optimization, and performance prediction. The research scope covers diverse material systems ranging from atomic and molecular scales to macroscopic scales. Major product forms include cloud-based SaaS platforms, on-premises deployment software, materials informatics platforms, and application programming interface services. The underlying technological processes involve materials database construction, feature engineering, high-throughput computational screening, molecular dynamics simulation, multi-scale simulation, and predictive model training and deployment. Key functionalities include inverse material design, formulation optimization, synthesis pathway planning, intelligent experimental data analysis, and R&D decision support. The software is widely applied in the rapid discovery and industrial development of advanced materials, including new energy battery materials, semiconductor electronic materials, metal alloys, polymer materials, catalysts, and pharmaceutical intermediates.

Global materials R&D is shifting from trial-and-error experimentation in the lab to a more systematic, data and AI driven approach. Over the past several years, the accumulation

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of computational and experimental materials data upstream, combined with the maturing of AI algorithm frameworks midstream, has directly translated into actual purchasing decisions by corporate R&D departments downstream for AI materials software. Looking at the product landscape, the industry has converged around three major technical categories: materials informatics platforms that mine data to identify patterns, machine learning interatomic potential platforms that use AI to replace first principles calculations for ultrafast simulations, and generative materials design platforms that directly propose candidate structures. Each category has its own trade offs, with some more dependent on data volume, others prioritizing physical interpretability, and still others focused purely on computational throughput. Meanwhile, governments across North America, Europe, and Asia have been rolling out programs around materials genome engineering and AI for Science, which is pushing more companies and research institutes to actually pay for these software tools, creating real growth headroom for the industry.

From a competitive landscape perspective, North America got the earliest start with a mature software ecosystem and venture capital system, producing a wave of platform companies built on AI technology as their core moat. Europe's advantage lies in its deep foundational research in chemistry and materials, giving it distinctive strength in generative materials modeling. On the Asian side, Chinese companies have made notable progress in developing localized materials databases and industry specific models, with fast product iteration and quick customer response as their key competitive edge. One trend worth watching is that several of the established players in traditional materials simulation are now adding AI modules to their software either through internal development or acquisitions. This means competition has expanded from a race among a handful of startups to a broader battle across the entire materials software ecosystem.

Looking ahead, whether this industry can sustain its growth comes down to two things. First, whether AI models can generalize to cover a wider range of material systems, allowing the same platform to handle more diverse R&D tasks. Second, whether materials data infrastructure can become more standardized, breaking down the current data silos and lowering the barrier to entry for new users. Global R&D spending on sustainable energy, advanced manufacturing, and lightweight materials continues to intensify, providing clear demand anchors for AI materials software. While challenges remain, such as inconsistent data quality and the long time required to build customer trust, the value of AI materials software in shortening R&D cycles and reducing experimental costs has already been validated by numerous real world cases. Over the next five to eight years, this industry will maintain a steady, sustainable expansion trajectory.

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This report is a detailed and comprehensive analysis for global AI-driven Materials R&D Software market. Both quantitative and qualitative analyses are presented by company, by region & country, by Function and by Application. As the market is constantly changing, this report explores the competition, supply and demand trends, as well as key factors that contribute to its changing demands across many markets. Company profiles and product examples of selected competitors, along with market share estimates of some of the selected leaders for the year 2025, are provided.

Key Features:

Global AI-driven Materials R&D Software market size and forecasts, in consumption value ($ Million), 2021-2032

Global AI-driven Materials R&D Software market size and forecasts by region and country, in consumption value ($ Million), 2021-2032

Global AI-driven Materials R&D Software market size and forecasts, by Function and by Application, in consumption value ($ Million), 2021-2032

Global AI-driven Materials R&D Software market shares of main players, in revenue ($ Million), 2021-2026

The Primary Objectives in This Report Are:

To determine the size of the total market opportunity of global and key countries

To assess the growth potential for AI-driven Materials R&D Software

To forecast future growth in each product and end-use market

To assess competitive factors affecting the marketplace

This report profiles key players in the global AI-driven Materials R&D Software market based on the following parameters - company overview, revenue, gross margin, product portfolio, geographical presence, and key developments. Key companies covered as a part of this study include Citrine Informatics, Preferred Computational Chemistry (Matlantis), MaterialsZone, Kebotix, Exabyte.io, DP Technology, XtalPi, Uncountable,

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QuesTek Innovations, CuspAI, etc.

This report also provides key insights about market drivers, restraints, opportunities, new product launches or approvals.

Market segmentation

AI-driven Materials R&D Software market is split by Function and by Application. For the period 2021-2032, the growth among segments provides accurate calculations and forecasts for Consumption Value by Function and by Application. This analysis can help you expand your business by targeting qualified niche markets.

Market segment by Function

Materials Discovery

Inverse Materials Design

Formulation Optimization

Molecular Simulation

High-throughput Screening

Experimental Data Analytics

Synthesis Pathway Planning

Others

Market segment by Computing Capacity

Small-scale Computing Capacity Below 100 TFLOPS

Medium-scale Computing Capacity 100–1000 TFLOPS

Large-scale Computing Capacity Above 1000 TFLOPS

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Market segment by Throughput

Low-throughput Screening Below 10 Thousand Candidates per Day

Medium-throughput Screening 10 Thousand–1 Million Candidates per Day

Ultra-high-throughput Screening Above 1 Million Candidates per Day

Market segment by Application

Energy and Power

Electronics and Semiconductors

Automotive and Transportation

Chemicals and Advanced Materials

Pharmaceuticals and Healthcare

Others

Market segment by players, this report covers

Citrine Informatics

Preferred Computational Chemistry (Matlantis)

MaterialsZone

Kebotix

Exabyte.io

DP Technology

XtalPi

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Uncountable

QuesTek Innovations

CuspAI

Polymerize

Market segment by regions, regional analysis covers

North America (United States, Canada and Mexico)

Europe (Germany, France, UK, Russia, Italy and Rest of Europe)

Asia-Pacific (China, Japan, South Korea, India, Southeast Asia and Rest of Asia-Pacific)

South America (Brazil, Rest of South America)

Middle East & Africa (Turkey, Saudi Arabia, UAE, Rest of Middle East & Africa)

The content of the study subjects, includes a total of 13 chapters:

Chapter 1, to describe AI-driven Materials R&D Software product scope, market overview, market estimation caveats and base year.

Chapter 2, to profile the top players of AI-driven Materials R&D Software, with revenue, gross margin, and global market share of AI-driven Materials R&D Software from 2021 to 2026.

Chapter 3, the AI-driven Materials R&D Software competitive situation, revenue, and global market share of top players are analyzed emphatically by landscape contrast.

Chapter 4 and 5, to segment the market size by Function and by Application, with consumption value and growth rate by Function, by Application, from 2021 to 2032.

Chapter 6, 7, 8, 9, and 10, to break the market size data at the country level, with

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revenue and market share for key countries in the world, from 2021 to 2026.and AI-driven Materials R&D Software market forecast, by regions, by Function and by Application, with consumption value, from 2027 to 2032.

Chapter 11, market dynamics, drivers, restraints, trends, Porters Five Forces analysis.

Chapter 12, the key raw materials and key suppliers, and industry chain of AI-driven Materials R&D Software.

Chapter 13, to describe AI-driven Materials R&D Software research findings and conclusion.

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