XtalPi: Defining the Next-Generation R&D Paradigm Through AI for Science

Boston, Massachusetts May 22, 2026 (Issuewire.com**)** - The methods that drive scientific discovery are undergoing a quiet but substantial transformation. Empirical, iterative experimentation has driven extraordinary progress across biopharma, advanced materials, and energy, yet the scale and complexity of contemporary research questions are placing growing demands on these established methods. AI for Science (AI4S) has emerged as a complementary paradigm that augments human expertise: by applying machine learning and deep learning to large experimental datasets and complex physical phenomena, researchers can extract patterns, build predictive models, and accelerate the journey from hypothesis to validated discovery. In doing so, AI4S offers new ways to bridge the well-known translational gap between fundamental insight and deployable technology.

Within this global shift, **XtalPi** has developed an integrated, closed-loop system that couples AI-driven prediction, robotic execution, data feedback, and multi-agent orchestration. In 2025, the company reached profitability—an early indication that AI4S is beginning to translate from conceptual promise into industrial value.

The R&D Flywheel: From Experimental Assistance to Autonomous Experimentation

At the heart of XtalPi's approach is a self-reinforcing R&D flywheel. Industrial research has long been shaped by the finite bandwidth of expert teams and the inherent latency of wet-lab cycles—constraints that even the most talented scientists cannot fully overcome on their own. By pairing AI-driven reasoning with robotic precision execution, XtalPi reframes the classical Design–Make–Test–Analyze (DMTA) cycle as a continuous, autonomous workflow. A multi-agent layer serves as the cognitive hub: it invokes domain-specific AI models to reason over candidate experiments, dispatches tasks to robotic laboratories, and ingests the resulting high-quality data back into the models. Predictions guide experiments; experiments generate data; data refine predictions—and each turn of the loop strengthens the next.

Multi-Agent Systems: From Human-Led Coordination to Autonomous Orchestration

In traditional research programs, a substantial portion of a scientist's time is spent on coordination, resource allocation, and troubleshooting—work that is necessary but often competes with the deeper scientific questions that only human judgment can frame. XtalPi's multi-agent system is designed to take on this operational layer, freeing researchers to focus on the problems where their expertise matters most.

Given a complex research objective, the system decomposes it into an executable task graph with explicit priorities and milestones, and coordinates with specialized AI models to support decision-making across the R&D chain. It allocates compute, instruments, and human–machine resources according to real-time availability, while monitoring experiments and model behavior to flag anomalies and initiate corrective actions. Experimental results are streamed back to the models to support continuous refinement, closing a loop of *model prediction → experimental validation → data feedback → model iteration*.

In drug discovery, XtalPi is building an end-to-end agent stack—**PatSight** for patent and literature intelligence, the **Vast™** virtual compound library, and synthesis robots coordinated by a central

scheduler. Together, these agents handle sourcing decisions, robotic execution, reaction-level decision-making, and data curation, drawing on dedicated AI models at each step. The system now autonomously advances tens of thousands of compound-synthesis experiments per week, accelerating chemical throughput and data accumulation across a tightly coupled pipeline of small-molecule design, high-throughput automated synthesis, and closed-loop data generation.

In this configuration, machines handle exploratory iteration and routine decisions, while scientists set top-level objectives and make the judgment calls that shape a program's direction. The researcher's role shifts from executing experiments and managing logistics toward defining objectives and making the strategic calls that shape a program's direction—a transition that elevates, rather than displaces, scientific expertise.

AI Models: From Supporting Tools to Decision Partners

Drawing on years of close collaboration with industry partners, XtalPi has developed more than 200 domain-specific AI models spanning small molecules, biologics, and emerging modalities such as molecular glues, peptides, and siRNA. Drug discovery is a cross-scale, multi-stage, multi-objective optimization problem; XtalPi's model portfolio reflects that reality, covering the full path from target identification and molecular design to preclinical candidate selection.

These models combine domain knowledge and expert heuristics with physics-based inputs—most notably molecular dynamics simulations—embedding dynamic physical principles directly into the modeling framework. This combination complements individual expert intuition with systematic, physics-aware modeling, providing a stronger technical foundation for addressing targets that have historically been considered undruggable. Among XtalPi's flagship outputs, its generative AI platform for protein therapeutics has demonstrated competitive performance on community benchmarks and has been recognized within the industry.

Crucially, these models do not sit in isolation. They receive real-time experimental feedback from XtalPi's robotic laboratories and are continuously refined under multi-agent orchestration. Originally developed for drug discovery, this model ecosystem and intelligent R&D paradigm is now being extended to materials, energy, and other frontier domains.

Robotic Laboratories: Bringing AI into the Physical World

AI model performance depends on high-quality data at scale—a requirement that manual experimentation, even when performed with great care, is inherently difficult to meet across the volume, standardization, and precision that modern models demand. An algorithm that never makes contact with the physical world cannot, on its own, deliver on the promise of AI for Science.

XtalPi's automated robotic laboratories serve as the bridge between computation and the physical world. Through a **Physical AI** stack that integrates physical laws, experimental mechanisms, and machine learning—together with advanced visual perception and specialized predictive models—the system achieves high reproducibility with minimal experimental error and enables high-throughput automated execution for approximately 80% of common chemical reactions. The footprint now spans chemical synthesis, biological screening, and materials preparation: synthesis robots operate 24/7 and complete tens of thousands of reactions per week; high-throughput screening platforms compress workflows from weeks to hours; and a new-energy-materials platform realizes a seamless loop of digital design, physical validation, and data feedback.

The high-quality, multimodal datasets generated by these platforms are integrated with literature and computational data into a unified data asset—a curated, standardized, domain-specific data foundation that fuels the continuous improvement of XtalPi's AI models.

Industrial Validation: From Undruggable Targets to Next-Generation Energy

In 2025, XtalPi's autonomous experimentation platform contributed to a series of program-level milestones in life sciences. Through deepening collaborations with global pharmaceutical companies, including Pfizer and Eli Lilly, its AI models have shown strong performance on protein–protein interaction (PPI) targets that have long been considered difficult to drug with small molecules.

At the pipeline level, **SIGX1094**, co-developed with **Signet Therapeutics**, has entered clinical trials as a first-in-class targeted therapy for diffuse-type gastric cancer and received a 2025 Prix Galien nomination—an early external validation of the organoid-plus-AI discovery model. In rare-disease drug development, XtalPi's collaboration with **ReviR Therapeutics** supported the **RTX-117** program, an oral small-molecule eIF2B activator that modulates the integrated stress response (ISR) pathway and has secured parallel IND clearances in the United States and China for Charcot–Marie–Tooth disease (CMT).

Beyond biopharma, XtalPi is extending its AI4S foundations into broader industrial domains. In consumer health, its proprietary hair-growth molecule has received INCI registration. In new energy, a strategic partnership with **JinkoSolar** aims to build the first AI-driven, closed-loop manufacturing line for tandem solar cells.

Closing Perspective

Under the AI4S paradigm, discovery relies less on serendipity alone. When mechanistically informed AI models operate alongside automated experimental platforms, cross-disciplinary innovation can be pursued with greater systematicity—while preserving the deep human expertise that defines scientific judgment.

As one of the leading companies in AI for Science, XtalPi continues to explore the boundaries of what AI4S can accomplish—embedding AI-driven autonomous experimentation across drug discovery, new energy, and materials science, and integrating computation, experimentation, and intelligent orchestration into a mature, market-validated R&D paradigm. In life sciences, the goal is to accelerate the discovery of new medicines and contribute to longer, healthier human lifespans; in energy and materials, to help push past performance ceilings and broaden the boundaries of sustainable development. By combining efficiency, precision, and a lower-carbon experimental footprint, XtalPi's autonomous experimentation platform points toward a new model for how scientific and technological innovation can be pursued.

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