Enthought

References & Resources

Agentic AI in Scientific R&D

As of September 2025

Agentic AI x Science

As autonomous AI systems become more sophisticated, scientists and R&D teams are seeking guidance on how these technologies can be applied to research challenges. Enthought's experts have compiled this reference guide to help navigate the emerging landscape of agentic AI.

> On-demand webinar
> **Making Sense of Agentic AI: A Strategic Briefing for Materials & Chemistry R&D Leaders**
> https://www.enthought.com/webinar-agentic-ai-in-materials-chemistry-2025

Further Reading About How Science and R&D are Changing

While AI continues to revolutionize scientific research, agentic AI is transforming R&D organizations themselves. Companies are integrating AI co-scientists that can generate hypotheses, design experiments, and validate results across fields. Instead of just being intern-level assistants, these agentic AI systems are now full-fledged PhD-level research partners that can conduct independent scientific investigations, further accelerating the pace of discovery and innovation.

- **Agentic AI for Scientific Discovery: A Survey of Progress, Challenges, and Future Directions** - Agentic AI systems are transforming scientific discovery by autonomously performing complex research workflows, with demonstrated success in chemistry, biology, and materials science.
- **AI, agentic models and lab automation for scientific discovery — the beginning of scAInce** - Reviews the transition from AI as a research co-pilot to autonomous "lab-pilot" systems that orchestrate both literature review and laboratory execution.
- **From AI for Science to Agentic Science: A Survey on Autonomous Scientific Discovery** - How AI is evolving from specialized computational tools into autonomous research partners capable of hypothesis generation, experimental design, execution, and analysis across life sciences, chemistry, materials science, and physics.
- **The Future of Material Scientists in an Age of Artificial Intelligence** - Explores how increasingly sophisticated AI systems are changing materials science research and what new skill sets researchers will need to stay competitive, using an "AI-ladder" framework.
- **A Survey of AI for Materials Science: Foundation Models, LLM Agents, Datasets, and Tools** - AI foundation models are transforming materials science by moving beyond traditional narrow AI to systems that can work across different domains and show new capabilities, covering six key areas.
- **Applied Artificial Intelligence in Materials Science and Material Design** - Examines practical AI implementations currently being deployed in materials research laboratories, focusing on how machine learning algorithms are being introduced into existing workflows to improve synthesis processes and predict material properties.
- **SciAgents: Agentic AI for discovery** - Introduces AI systems capable of autonomously advancing scientific understanding by exploring different domains, identifying complex patterns, and uncovering previously unseen connections in datasets.

Enthought

General Tools for Learning

We recommend trying out agentic AI tools to get a baseline understanding of how they work and get a sense of their potential when applied at the enterprise level.

Agentic AI Tools

- **OpenAI -** https://openai.com/index/new-tools-for-building-agents/
  OpenAI is developing comprehensive tools for building agentic AI systems, including their Agents SDK for developers and consumer products like Operator that can autonomously perform multi-step tasks in digital environments.

- **CrewAI** - https://www.crewai.com/
  CrewAI is a Python framework for building teams of AI agents with specialized roles that collaborate to complete complex tasks.

- **E2B -** https://e2b.dev/
  E2B is an open-source runtime for executing AI-generated code in secure cloud sandboxes, designed specifically for agentic AI applications.

- **Anthropic -** https://www.anthropic.com/solutions/agents/
  Anthropic advocates for "simple, composable patterns" over complex frameworks with a focus on building agents through workflows and autonomous systems that use tools and environmental feedback to accomplish tasks independently.

- **AI Agents for Beginners -** https://github.com/microsoft/ai-agents-for-beginners
  Microsoft's "AI Agents for Beginners" is a free educational course that teaches the fundamentals of building AI agents.

- **Cursor** - https://cursor.com/
  Cursor is an AI-native code editor designed to make writing and understanding code faster and more efficient.

Protocols

- **Model Context Protocol (MCP)** - https://www.anthropic.com/news/model-context-protocol
  Anthropic's MCP standardizes the interaction between large language model (LLM)-based agents and external tools or APIs.

- **Agent Communication Protocol (ACP) -** https://agentcommunicationprotocol.dev/introduction/welcome
  The ACP is an emerging open standard designed to enable interoperability between different AI agents, regardless of their underlying frameworks, technologies, or developers.

- **Universal Tool Calling Protocol (UTCP)** - https://www.utcp.io/utcp-vs-mcp
  The UTCP is an open standard, as an alternative to the MCP, that describes how to call existing tools rather than proxying those calls through a new server.

- **Agent2Agent (A2A) -** https://developers.googleblog.com/en/a2a-a-new-era-of-agent-interoperability/
  Google's A2A provides a structured JSON-over-HTTP approach for agent-to-agent communication, supporting clearly defined task lifecycles and real-time communication via SSE (Server-Sent Events) or webhooks