



# Foundation Models for Materials Design and Autonomous Synthesis

Program Solicitation NSF 26-534

|                        |                            |
|------------------------|----------------------------|
| Full Proposal Deadline | March 17, 2026             |
| Letter of Intent       | Not required               |
| Award Size             | \$1,200,000 total, 3 years |
| Anticipated Awards     | 8 to 12                    |
| Cost Sharing           | Required — 25% non-federal |

## Synopsis

This solicitation supports the development of **foundation models**, **machine learning** and **agentic AI** methods for the design, prediction and autonomous synthesis of **inorganic and polymeric materials**. Proposals should advance representation learning over crystal structures, reaction networks and process parameters, and should demonstrate closed-loop integration with automated synthesis platforms.

Topics of interest include **large language model** agents for literature-driven hypothesis generation, **AI-ready datasets** and benchmarks for materials property prediction, **continual learning** under distribution shift as instruments drift, and **deep learning** surrogates for first-principles simulation.

## Scope

**Out of scope.** Proposals whose primary application domain is the life sciences — including genomics, structural biology, protein or nucleic acid modelling, plant science, agriculture, or biomedical applications — are **not responsive** to this solicitation and will be returned without review. The Directorate for Biological Sciences and the Directorate for Biological Infrastructure support such work through separate programs.

Materials of interest: catalysts, battery electrodes and electrolytes, structural alloys, semiconductors and photonic materials, and functional polymers.

## Cost Sharing

**Cost sharing of 25% of the total project cost from non-federal sources is required** and must be documented in a letter from the authorized organizational representative at the time of submission. Proposals without a documented commitment will be returned without review. In-kind contributions may be counted only where independently valued.

## Eligibility

IHEs and non-profit research organizations. No limit on submissions.