

Schmidt Sciences

2026 AI for Actionable Matter Modelling RFP

Opens Feb 13 2026 12:00 AM (EST)

Deadline Apr 30 2026 11:59 PM (EDT)

Description**Request for Proposals: AI for Actionable Matter Modeling**

This is a pilot program. We are exploring whether AI-driven methods can reliably predict the material and molecular properties that determine technological function in the real world—defects, interfaces, disorder, and dynamics operating at multiple length and time scales. If this pilot uncovers compelling evidence, it may unlock a significantly larger, multi-year investment in this space.

This is a lightweight application. There are no letters of support, no spreadsheets to be filled. The application consists of a short online form and a (less than) 5-page project narrative pdf. We're interested in what you've built and where you want to take it—not your ability to write long proposals.

Overview

Fields that manipulate matter—chemistry, materials science, biology—face a persistent gulf between computational models and the lab bench. Conventional simulation emphasizes idealization: perfect crystal structures, static snapshots, vacuum environments, and single length or time scales treated in isolation. But the functional properties of foundational technologies (catalysts, semiconductors, drugs, batteries) are determined by non-idealities—defects, interfaces, disorder, dynamics—operating across scales that conventional methods cannot connect. As Nobel Laureate Herbert Kroemer remarked of semiconductors, "the interface is the device."

We believe that AI may now help close this gap—not only by modeling non-idealities more accurately at a single scale, but by bridging scales that have historically required separate communities, codes, and assumptions. We are equally interested in methods that improve fidelity within a single scale and methods that connect scales that today are treated in isolation. We want simulations to move from post-hoc explanations to credible guidance that experimentalists use to decide what to synthesize or measure next.

This RFP is for you if:

- You are developing AI methods to predict non-idealities (defects, interfaces, disorder, dynamics)

APPLY