Received: May 29, 2025
Tracking No. mb9-7pfs-ywgq
Comments Due: May 28, 2025 **Submission Type:** Web

PUBLIC SUBMISSION

Docket: NSF-2025-OGC-0001
NITRD_FRDOC_0001

Comment On: NSF-2025-OGC-0001-0001
Request for Information: Development of a 2025 National Artificial Intelligence Research and Development Strategic Plan

Document: NSF-2025-OGC-0001-DRAFT-0174
Comment on FR Doc # 2025-07332

Submitter Information

Name: Niloofar Yousefi

General Comment

See attached file(s)

Attachments

RFI_Response_Yousefi

Response to RFI: 2025 National AI R&D Strategic Plan

Introduction

The transformative potential of artificial intelligence in **national security, healthcare, and scientific innovation** lies not only in its predictive capacity but in its ability to **drive the complete lifecycle of discovery**—from understanding to generation to deployment. **My research program aims to develop AI systems that operate across this full spectrum** by integrating theoretical understanding, predictive modeling, and responsive nanotechnology.
These capabilities are especially critical for strategic applications such as **rapid therapeutic development**, **targeted delivery under extreme conditions**, and **autonomous design of functional materials** for **biodefense and environmental resilience**.

Strategic Motivation and National Relevance

To remain globally competitive and secure, the U.S. must invest in **AI systems that enable rapid, data-driven responses** to evolving biological, chemical, and physical threats.
In **pandemic preparedness**, **warfighter health**, and **adaptive materials for defense**, there is an urgent need for AI that can:

1. **Identify and optimize effective compounds or materials**,
2. **Tailor delivery methods to dynamic contexts**, and
3. **Generalize reliably across settings**.

These challenges are **beyond the scope of commercial incentives** and demand **foundational, interdisciplinary AI research supported by the federal government**.

Integrated Research Vision

My research program is designed around a unified goal: enabling AI systems to reason end-to-end across the discovery and delivery of therapeutic and functional materials.
This goal is grounded in strong **interdisciplinary collaborations**—with material scientists, biologists, and engineers—and anchored in three complementary lines of work that collectively bridge **prediction**, **deployment**, and **theoretical understanding**.

First, my foundational work in **drug–target interaction (DTI) prediction** provides mechanistic insight into molecule–protein interactions, helping identify bioactive compounds with high therapeutic potential.
These models are built to be **interpretable and structure-aware**, ensuring not only predictive accuracy but also biological plausibility.
During the early COVID-19 pandemic, this approach led to the identification of several candidate treatments—including **Remdesivir**, which was later **FDA-approved—demonstrating the power of computational models to accelerate real-world biomedical discovery**.

Second, to translate discovery into application, my lab collaborates with experimentalists to develop **AI-designed nanobubbles—**nanoscale delivery vehicles that can respond to environmental stimuli such as pH or ultrasound.
These systems provide a **physical mechanism for targeted drug deployment** to precise tissue environments, including hypoxic regions or inflammation zones.
Their **adaptability makes them promising tools for battlefield medicine, disaster response, and personalized healthcare**, positioning this work within **emerging national security and biodefense priorities**.

Third, underpinning these advances is my lab's theoretical research on the **learning dynamics of large language models (LLMs)**.
We investigate how transformers **compress, propagate, and generalize information across domains—**a necessary step for developing **multi-modal, generative AI systems**.
These systems unify **symbolic, structural, and biochemical data**, enabling the **generation of new compounds or nanocarriers tailored for specific use-cases**.
This foundational work ensures that the models we build are not only **effective**, but also **principled**, **interpretable**, and **adaptable across scientific modalities**.

Together, these three components—target identification, intelligent delivery via nanobubbles, and theoretical insights into LLMs—form an integrated strategy for AI-driven scientific discovery.
They provide a pipeline that:

- Begins with **identifying what to deliver**,
- Proceeds through **designing how and where to deliver it**,
- And is guided throughout by a **rigorous understanding of why these models work**.

This approach represents a scalable and secure foundation for the next generation of AI systems serving **healthcare**, **biodefense**, and **material innovation**.

Recommendations for Federal AI R&D Investment

1. Support cross-disciplinary research between AI and scientific domains to drive high-impact, experimentally grounded discovery.
What it means:
Fund initiatives that promote deep collaboration between AI researchers and scientists across fields such as biology, medicine, and materials engineering, enabling the development of models that align with scientific needs and operational contexts.

Why it's important:
Scientific discovery is most effective when AI methods are paired with domain knowledge. These partnerships close the gap between algorithmic innovation and real-world application, yielding faster and more reliable outcomes.

2. Prioritize AI systems that support rapid response in national security scenarios such as biothreats or critical infrastructure resilience.
What it means:
Invest in AI platforms that can adapt quickly to emerging threats—like pandemics, chemical exposure, or supply chain disruptions—by guiding strategic decisions, generating countermeasures, or optimizing logistical responses.

Why it's important:
AI systems like the ones my team developed for COVID-19 drug repurposing have demonstrated how rapid, computationally guided insights can accelerate real-world impact. Federal support can ensure these capabilities are scalable, secure, and deployable during national emergencies.

3. Fund foundational research on LLM architectures tailored for multi-modal reasoning in materials and therapeutics.
What it means:
Support basic research into large language models (LLMs) that can reason across multiple data types—text, molecular structures, imaging, and graphs—especially in domains like drug discovery and materials science.

Why it's important:
LLMs hold potential for not just NLP, but also for generative design, cross-domain synthesis, and scientific reasoning. However, to be useful in scientific domains, they must be grounded in domain-specific theory and built for interpretability and trust.

Conclusion

This integrated research program bridges theory, modeling, and deployment to create AI systems that are capable not just of discovering new knowledge, but of acting on it. By supporting this type of high-risk, high-reward AI research, the federal government can accelerate breakthroughs that ensure U.S. leadership in health security, materials innovation, and AI-driven scientific advancement.

Submitted by: Dr. Niloofar Yousefi, University of Central Florida