DMREF: Designing Materials to Revolutionize and Engineer our Future

NSF 23-530: Informational Briefing

John Schlueter

Program Director National Science Foundation January 18, 2023

JSchluet@nsf.gov

(DMREF) PROGRAM SOLICITATION NSF 23-530 **REPLACES DOCUMENT(S):** NSF 21-522 National Science Foundation Directorate for Mathematical and Physical Sciences Division of Materials Research ivision of Chemistry ision of Mathematical Sciencer sion of Civil, Mechanical and Manufacturing Innovation vision of Electrical, Communications and Cyber Systems sion of Chemical, Bioengineering, Environmental and Transport System ce of Advanced Cyberinfrastructure sion of Computer and Network Syste ision of Information and Intelligent Systems Directorate for Technology, Innovation and Partnerships Innovation and Technology Ecosystems Ir Force Research Laboratory Ir Force Office of Scientific Research National Institute of Standards and Technology NIST Department of Energy (DOE) Office of Energy Efficiency & Renewable Energy Office of Naval Research U.S. Army Combat Capabilities Development Command - Army Research Laboratory U.S. Army Combat Capabilities Development Command - Ground Vehicle Systems Center Submission Window Date(s) (due by 5 p.m. submitter's local time) February 27, 2023 - March 13, 2023

Designing Materials to Revolutionize and Engineer our Future



Format and Agenda

Presentation of Solicitation information

- Introduction to the Materials Genome Initiative
- DMREF objectives
- Solicitation requirements
- Changes from previous years
- Question and Answer
 - Ask questions through Q&A box
 - Questions can be anonymous
 - Refer to slide number, if appropriate
 - Specific questions about your proposal should be addressed to DMREF Management Team members

This Webinar will be recorded and made publicly available. (Check DMREF.org following the webinar.)







Synopsis of DMREF Solicitation

- DMREF supports activities that significantly accelerate the materials discovery-touse timeline by building the fundamental knowledge base needed to advance the design, development, or manufacturability of materials with desirable properties or functionality.
- > Achieving this goal could involve some combination of:
 - Strategies to advance fundamental knowledge of materials design and manufacturability,
 - Theory, computation/simulation, and modeling that leverage machine learning, artificial intelligence, data mining, or sparce approximation to predict materials behavior,
 - Automated, high-throughput, and/or autonomous experimentation, including cyber-physical systems, that streamline and optimize the search of materials space
 - Validation through synthesis, growth, processing, characterization and/or device demonstration.



Important Information and Revision Notes

- NSF Solicitation number: 23-530
- Submission window: February 27-March 13, 2023
 - Proposals due by 5 PM submitter's local time Late proposals will be returned without review!
- Next competition: 2025 (biennial program)
- > Award size/duration: \$1.5-\$2.0 M over 4 years
- > Size of team: Minimum of 2 PIs, Typically 3-5 PIs
- > 10 NSF divisions will participate in 2023



- Includes Division of Innovation and Technology Ecosystems (ITE) in Directorate for Technology, Innovation and Partnership (TIP)
- Additional federal agencies will partner with DMREF in 2023
- Partnerships with industry are encouraged (i.e., GOALI)
- Proposals led by or including Minority Serving Institutions (MSI) or Primarily Undergraduate Institutions (PUI) are encouraged
 - DMREF encourages efforts to promote diversity, inclusion, equity, and accessibility and advance environmental justice
- Proposals must have a Data Management Plan that is responsive to findable, accessible, interoperable, and reusable (FAIR) data practices.



DMREF Management Team

These are your primary contacts for DMREF-related questions!

Computer and Information CISE Science and Engineering



Andrey Kanaev OAC



Jim Donlon IIS



Ralph Wachter **CNS**



Suk-Wah Tam-Chang CHE

Eugenia **Kharlampieva** DMR



Tiziana

Giorgi

DMS

MATERIAL



John **Schlueter** DMR



Marian Bocea DMS

Mohsen Asle Zaeem DMR

Mathematical and

Physical Sciences



Gorb

DMS

Yuliya



Paul

Lane

Bob **McCabe** CBET





Siddig

Qidwai

CMMI



Richard Nash **ECCS**



Shahab Shojaei-Zadeh CBET



Leon **Shterengas ECCS**



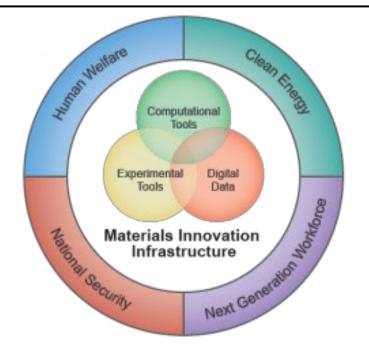
Designing Materials to Revolutionize Our Engineering Future

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Materials Genome Initiative (MGI)

Established June 2011

Mission: To help businesses discover, develop, and deploy new materials twice as fast at a fraction of the cost.



DMREF is NSF's primary response to the MGI



Goals of the Materials Genome Initiative

- A paradigm shift has occurred.
- Unify the Materials Innovation Infrastructure.
- Harness the power of materials data.
- Educate, train, and connect the Materials R&D workforce.





Federal MGI Partners

Coordination of MGI-related efforts is critical to success.



DMREF encourages partnerships with other federally funded MGI efforts.

- Desire integrated Materials Innovation Infrastructure
- Need a single National Materials Data Network



Formal Partnerships between DMREF and Federal Agencies















Air Force Research Laboratory Contact: Ruth Pachter <u>RuthPachter@us.af.mil</u>

Air Force Office of Scientific Research Contact: William Roach <u>William.Roach.4@us.af.mil</u>

National Institute of Standards and Technology Contact: James Warren <u>James.Warren@nist.gov</u>

Department of Energy Office of Energy Efficiency & Renewable Energy Contact: Eric Miller <u>Eric.Miller@ee.doe.gov</u>

Office of Naval Research Contact: Knox Millsaps <u>Knox.T.Millsaps.civ@us.navy.mil</u>

U.S. Army Combat Capabilities Development Command – Army Research Laboratory Contact: Adam Rawlett <u>Adam.M.Rawlett@army.mil</u>

U.S. Army Combat Capabilities Development Command – Ground Vehicle Systems Center Contact: David Gorsich <u>David.J.Gorsich.civ@army.mil</u>



Considerations for Including Federal Partners

- Partnerships are not required, and no funding preference will be given to proposals simply because of collaboration with federal partners.
- > Partnerships may:
 - Bolster the scientific aspects of the iterative feedback loop to accelerate materials research.
 - Facilitate the translation of fundamental materials research toward application.
 - Provide education, training, and workforce development opportunities.
- > Do not list federal personnel on the Cover Page.
 - Note: GOALI partners must be listed on Cover Page.
- > Federal PIs may participate in more than one DMREF proposal.
- > If involving DMREF federal partners, use Keywords: AFRL, EERE, ONR, NIST, GVSC, or ARL
- > Letters of Collaboration are not required from DMREF's federal partners.
- > Collaborations with other federal agencies (NASA, NIH, etc.) are allowed.

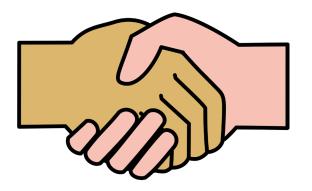


Further Considerations for Including Federal Partners

- Project Description:
 - Must identify the collaborating PI and thoroughly explain how this collaboration will benefit both the DMREF team and the federal partner in advancing the goals of the project.

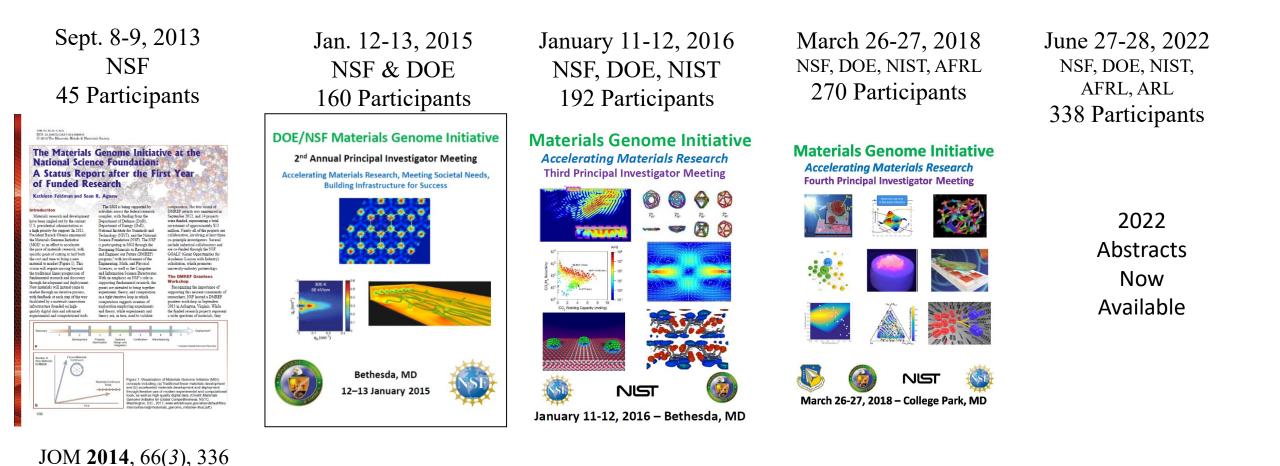
Management Plan

- Must describe how collaborative activity would be implemented and integrated.
- > Budget:
 - May include funds such as to support PI or student travel to enable these activities.
 - No funds may be budgeted or sub-awarded to federal partner.
- > Specific interests of federal partners are found on page 8 of the solicitation.





Annual MGI PI Meeting



These proceedings provide a good summary of DMREF and MGI projects. Proceedings of 2022 meeting will be available soon.

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Designing Materials to Revolutionize Our Engineering Future

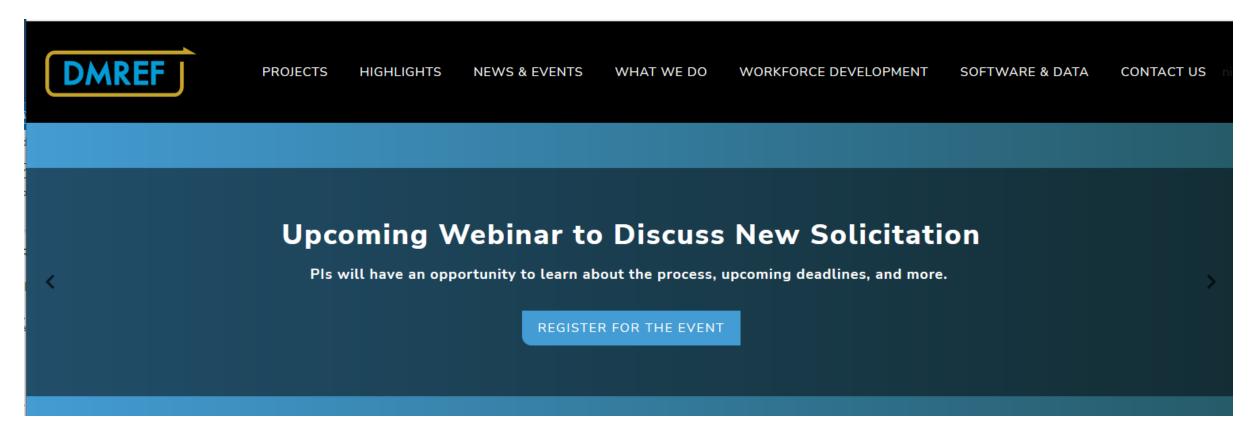
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Available at:

DMREF.org

DMREF.org

- Provides information to the DMREF community.
 DMREF project summaries, highlights, publications, etc.
- DMREF Matchmaker tool will be added later this month.





National Academies Study of DMREF

- > NASEM has evaluated the effectiveness of DMREF program in addressing the goals of MGI.
- > Report is freely available on-line.
- Provides a series of findings and recommendations for the future of DMREF.



NationalAcademies.org



DMREF Scope

DMREF encourages high-risk/high-payoff proposals where MGI principles can significantly accelerate progress.

- Covers all materials classes
- Aligns with national priorities
- Proposals from multidisciplinary teams
 - About 85% of DMREF proposals are co-funded by multiple NSF divisions
- It's not only the Material it's the Philosophy
 - Driving materials research through computation and data
- DMREF has a Mission
 - Accelerate translation of materials from design to deployment



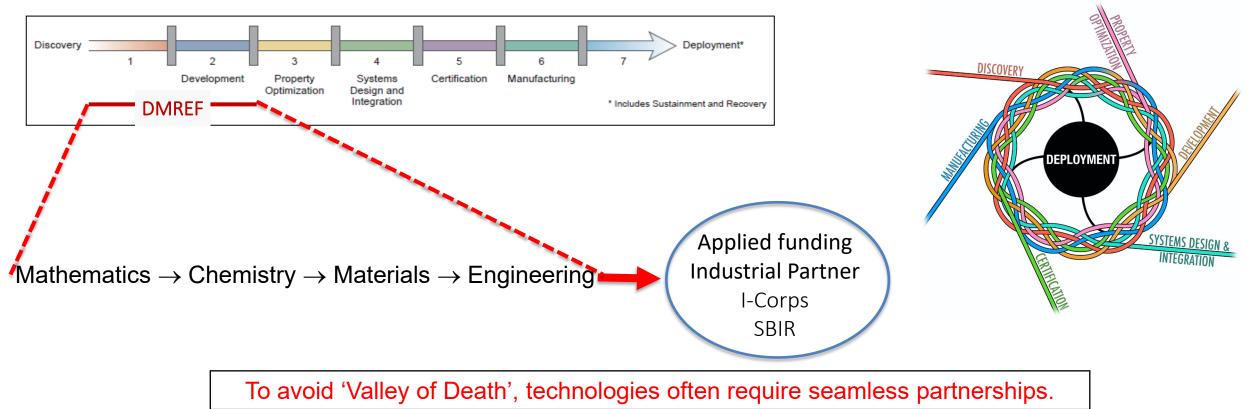


Materials Discovery to Deployment

Accelerating the progression of fundamental materials research toward eventual deployment and manufacturing.

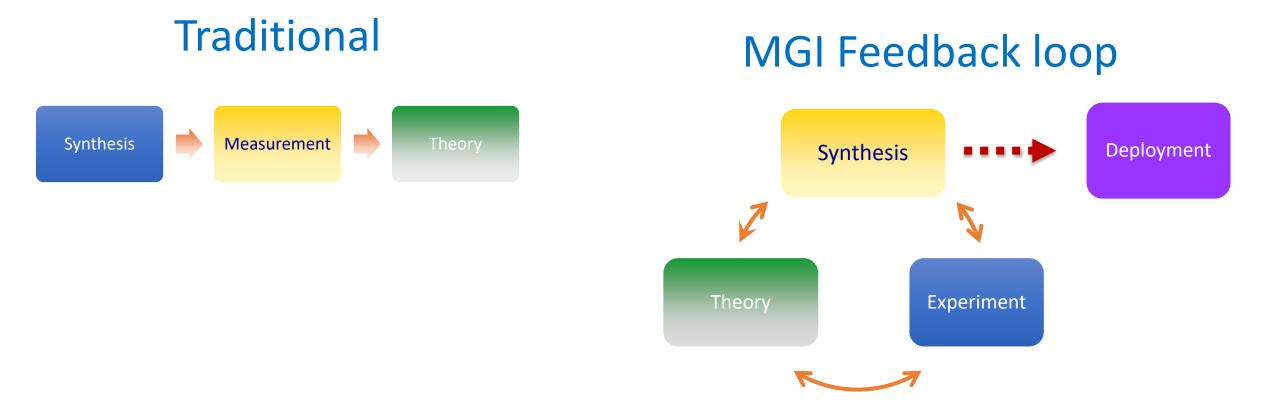
Materials Development Continuum

Materials Innovation Infrastructure





Research Progression

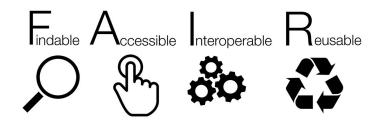


An effective iterative feedback loop is a key component of a DMREF team.



DMREF Data Management Plan

- See: MGI Strategic Plan Goal 2
 - Foster a National Materials Data Network
- Data Management Plan (DMP) will be reviewed
- FAIR data practices must be considered

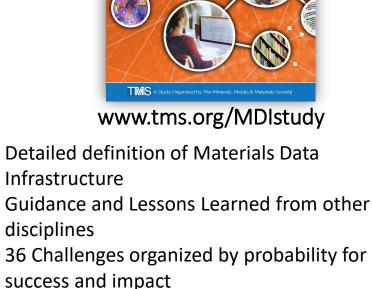


- Digital outputs include codes, computational and experimental data, training material, etc.
- Support for software engineers, database programmers, or other individuals is allowable in DMREF budgets.

DMREF Data Management Plan Guidance:

https://www.nsf.gov/bfa/dias/policy/dmpdocs/dmref.pdf



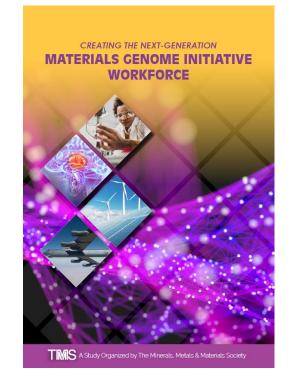


erials Data

- 8 recommendations with 22 detailed tactics
- Summary of 17 prior workshops and reports

Training the Next Generation Workforce

- See: MGI Strategic Plan Goal 3
 - Address current challenges in materials R&D education
 - Train the next generation materials R&D workforce
 - Connect Talent to Opportunity
- How will students associated with the project be trained in a multidisciplinary manner consistent with the MGI philosophy?
- What educational outreach activities will be pursued to engage K-12 (and other) students?
- How will the exciting technological aspects of the project be conveyed to the public?
- Workforce development should be a team effort, not a collection of individual efforts.



www.tms.org/MGIWorkforce

- Modernize academic curricula with MGI content
- Identify, develop, and package instructional modules
- Develop targeted short courses, boot camps, and summer schools



Accelerating MGI Research through AI

> MGI Strategic Plan:

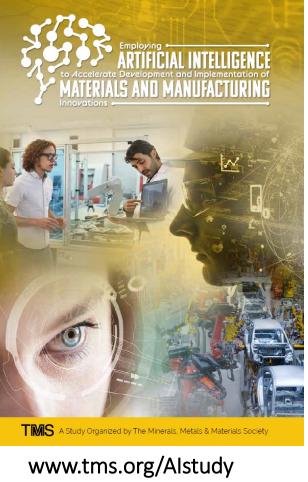
Accelerate Materials R&D Deployment through application of AI

- Relevant topics
 - Data analytics
 - Artificial intelligence (various flavors)
 - Automation, high-throughput, cyber-physical systems
 - Autonomous research
- May include partnerships with:
 - Mathematics
 - Statistics
 - Computer science

TMS study 'Artificial Intelligence for Materials and Manufacturing'

Describes 8 Action Plans





If Submitting a DMREF Proposal:

- Proposals may <u>only</u> be submitted by Institutions of Higher Education
- Indicate primary division with which proposal is most closely aligned
 - Projects don't need to be led by materials scientists (or DMR)
 - Management Team makes final decision of ownership
 - Secondary divisions may be chosen
- Must be collaborative
 - Minimum of 2 PIs (3-5 typical: theory, synthesis, experiment)
 - Single- or multi-institution
- > An individual is limited to being senior personnel on a single 2023 DMREF proposal
 - Current DMREF PIs are eligible to submit
 - Proposals submitted to other parts of NSF do not affect eligibility (provided content isn't duplicative)
- Contact a DMREF Management Team member with specific questions.

NSF proposals must be submitted through Research.gov or Grants.gov. Fastlane may no longer be used.



PIs with Prior or Existing DMREF Projects

- > All DMREF proposals are reviewed as <u>new</u> proposals.
- > Follow-on funding only considered when proposal describes:
 - Ambitions plans for advancing along materials development continuum
 - Significantly new research directions
- Results from Prior NSF Support must substantially address progress made under DMREF award
 - ✤ Intellectual Merit
 - Broader Impact
 - Data Management Plan
 - DMREF Review Criteria





DMREF Panels/Panelists

- > PIs are encouraged to include list of potential reviewers for their DMREF proposals
- Panel review is conducted by research topic, not selected division
 e.g., 'Metals', 'Biomaterials', 'Quantum Materials', etc.
- Some proposals will be reviewed in multiple panels because of cross-cutting topics
 e.g., 'Mathematics', 'Artificial intelligence', etc.
- > If you do not submit a DMREF proposal, please consider volunteering as a panelist!

Volunteer panelists:

Please email DMREF Program Director Mohsen Asle Zaeem <u>MZaeem@nsf.gov</u> with "I want to review for DMREF" in the subject line. Please enclose your CV and indicate your areas of expertise.





NSF Merit Review Criteria

Intellectual Merit

The potential to advance knowledge

Broader Impacts

The potential to benefit society and contribute to the achievement of specific, desired societal outcomes.

The following elements should be considered in the review:

- What is the potential for the proposed activity to:
 - ✤ <u>Advance knowledge</u> and understanding within its field or across different fields
 - <u>Benefit society</u> or advance desired societal outcomes
- To what extent do the proposed activities suggest and explore <u>creative</u>, <u>original</u>, <u>or potentially</u> <u>transformative concepts</u>?
- Is the plan for carrying out the proposed activities well-reasoned, well-organized, and based on a <u>sound rationale</u>? Does the plan incorporate a mechanism to <u>assess success</u>?
- > How well <u>qualified</u> is the individual, team, or institution to conduct the proposed activities?
- Are there adequate <u>resources</u> available to the PI (either the home institution or through collaboration) to carry out the proposed activities?



Additional DMREF Review Criteria

> How effectively does the proposed work:

- Accelerate materials discovery, understanding and/or development by building the fundamental knowledge base needed to progress toward designing and making materials with specific, desired functions or properties?
- use collaborative processes with iterative feedback between tasks?
- Iead to significant advances in all components of the project, including materials synthesis / growth / processing, materials characterization / testing, and theory / computation / simulations?
- Provide training (including data-related training) for the next generation of scientists and engineers, educated in a multidisciplinary, integrated experimental and computational approach to materials research?
- describe efforts to promote diversity, equity, and inclusion?
- Convey that the digital data generated by the project will be made freely available within a reasonable time from publication, without need to request to the investigator, in a way that is findable, accessible, interoperable, and reusable (FAIR)?
- >Additionally, for proposals submitted to DMS as the primary unit of consideration
 - How effectively does the proposed works seek new mathematical or statistical results that will advance the DMREF agenda?

See page 13 of the solicitation for additional details.



Results from Prior NSF Support

Deficiencies have resulted in DMREF proposals being returned without review!

- Required for each PI and co-PI with:
 - An award with end-date in the past 5 years
 - Any current funding (including any no-cost extensions)
- > For PIs with current or previous DMREF awards, the DMREF award is likely the most relevant.
- > The following information must be provided:
 - NSF award number, amount, period of support
 - Title of project
 - Summary of results
 - Intellectual Merit
 - Broader Impact
 - (DMREF criteria)
 - List of publications resulting from award
 - Evidence of access to research products and their availability (Data Management)

See: Proposal & Award Policies & Procedures Guide (PAPPG) section II.C.2.d.iii

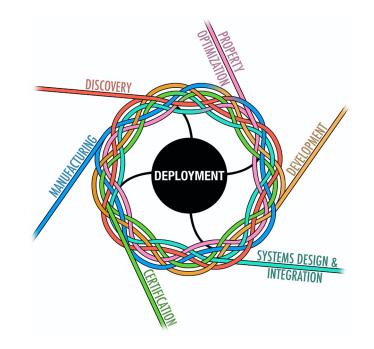


Grant Opportunities for Academic Liaison with Industry (GOALI)

DMREF recognizes the importance of partnerships among universities, industries, federal agencies and national and federal laboratories to achieve the goals of MGI.

For GOALI proposals:

- At least one industrial co-PI must be listed on the Cover Sheet
- University-industry interaction must be described in the Project Description
- Include GOALI-Industrial PI Confirmation Letter
- University-industry IP agreement required before issuance of award
- Non-SBIR small businesses are now allowed to receive funding as described in the PAPPG.
- Some projects may benefit from an industrial partner or industrial advisory board



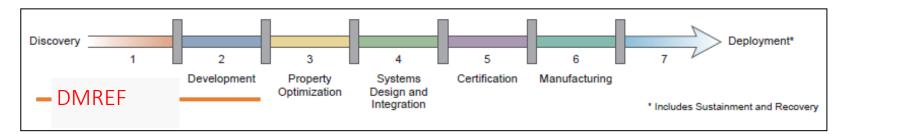
See: Proposal & Award Policies & Procedures Guide (PAPPG) section II.F.5



DMREF and Manufacturability

Consideration of the full range of material characteristics, properties, and manufacturing processes needed to attain the desired cost and performance of products is integral to achieving the ultimate goal of MGI.

- Where appropriate (i.e., depending on where a proposed project lies along the materials development continuum), DMREF proposals should consider manufacturability.
- 'Manufacturability' relates to properties relevant to manufacturing, process-property relationships, property performance metrics, scalable synthesis routes, economic feasibility, supply chain considerations, or life cycle issues.
- > DMREF-TIP seeks proposals that demonstrate technology:
 - Prototyping/validation transitioning to relevant practical environment.
 - Testing and/or demonstration at-scale in practical environment.

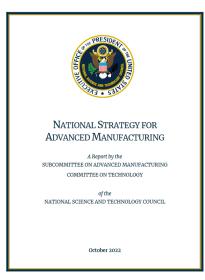








Siddiq Qidwai SQidwai@nsf.gov



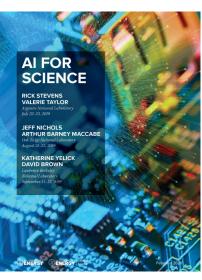
Artificial Intelligence in DMREF

- Use of AI tools are NOT required for DMREF
- Use of data tools has been growing rapidly and offers an opportunity to accelerate materials research.
- DMREF-IIS seeks proposals that present an ambitious plan for incorporating use-inspired or foundational AI into research plans.



Contact: Jim Donlon JDonlon@nsf.gov







RECOMMENDATIONS FOR STRENGTHENING AMERICAN LEADERSHIP IN INDUSTRIES OF THE FUTURE

A Report to the President of the United States of America The President's Council of Advisors on Science and Technology

June 2020



THE NATIONAL ARTIFICIAL INTELLIGENCE RESEARCH AND DEVELOPMENT STRATEGIC PLAN: 2019 UPDATE

A Report by the SELECT COMMITTEE ON ARTIFICIAL INTELLIGENCE of the NATIONAL SCIENCE & TECHNOLOGY COUNCIL

JUNE 201



Cloud Computing Resources

- Cloud computing resources may be obtained through Cloudbank.
- Request should be described in a 2-page Supplemental Document
 - Anticipated costs for necessary cloud computing resources
 - Identify which public cloud provider will be used
 - Amazon Web Services
 - Google Cloud Platform
 - IBM Cloud
 - Microsoft Azure
 - Technical justification for requested cloud computing resources
- > The total cost of the project, including cloud computing request, cannot exceed \$2.0 M.







Contact: Jim Donlon JDonlon@nsf.gov

Mathematical Sciences

Proposals considered for DMS co-funding will be co-evaluated for novelty of new mathematical and/or statistical advance benefitting DMREF/MGI goals.

Contact:



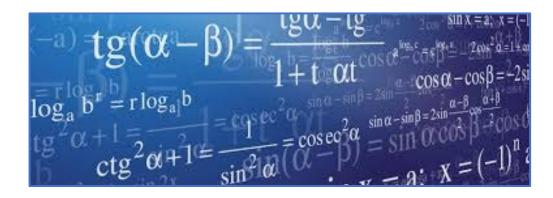
Tiziana Giorgi DMS



Marian Bocea DMS



Yuliya Gorb DMS





MATERIAL

Additional Considerations

> A Management Plan is required.

- Generally, more detail is required for proposals involving multiple institutions or federal partners.
- > The goal or objective of the project should be clearly stated.
- > A targeted property, structure, or function can often focus a proposal.
- > A defined figure-of-merit can be used to evaluate progress toward an ultimate goal.
- Proposed research must be substantially different from currently funded projects or proposals concurrently under consideration at NSF.





Take-home Message

- NSF Solicitation number: 23-530
- Submission window: February 27-March 13, 2023 (5 PM local!)
- > Award size/duration: \$1.5-\$2.0 M over 4 years
- > Size of team: Minimum of 2 PIs, Typically 3-5 PIs
- > Additional considerations:
 - ✤ Open to all areas of materials research: aligns with national priorities
 - ✤ 10 NSF divisions will participate (including Innovation and Technology Ecosystems)
 - New federal partners added; no preference given to proposals with federal partners
 - Partnerships with industry (GOALI) are encouraged
 - Where appropriate, manufacturability should be considered
 - Data Management Plan must be responsive to FAIR data practices
- > DMREF encourages high-risk/high-payoff proposals where MGI principles accelerate progress.
- DMREF doesn't require discovery of new materials
 - New processes, properties, functionality, etc. meet the requirement
- > DMREF encourages diversity, inclusion, equity, accessibility, and environmental justice.





Question and Answer Period



Type your questions into the Chat box. Include your name and email if you would like a personal response.

