Fiscal Year (FY) 2018 Department of Defense
Multidisciplinary Research Program of the University Research Initiative

Proposal Deadline
Your proposal must be received no later than **Wednesday, November 1, 2017 at 11:59 PM Eastern Daylight Time**

White Paper Deadline
Your white paper must be received no later than **Monday, July 17, at 11:59 PM Eastern Daylight Time**

Inquiries and Questions Deadlines
White Papers: Friday, June 30, 2017
Proposals: Wednesday, October 11, 2017

INTRODUCTION:

This publication constitutes a Funding Opportunity Announcement (FOA) as contemplated in the Department of Defense Grants and Agreements regulations (DoDGARS) 32 CFR 22.315(a). A formal Request for Proposals (RFP), solicitation, and/or additional information regarding this announcement will not be issued.

The Department of Defense (DoD) Multidisciplinary University Research Initiative (MURI), one element of the University Research Initiative (URI), is sponsored by the DoD research offices. Those offices include the Office of Naval Research (ONR), the Army Research Office (ARO), and the Air Force Office of Scientific Research (AFOSR) (hereafter collectively referred to as "DoD agencies").

DOD's MURI program addresses high risk basic research and attempts to understand or achieve something that has never been done before. The program was initiated over 25 years ago and it has regularly produced significant scientific breakthroughs with far reaching consequences to the fields of science, economic growth, and revolutionary new military technologies. Key to the program's success is the close management of the MURI projects by Service program officers and their active role in providing research guidance.

The DoD agencies will not issue paper copies of this announcement. The DoD agencies involved in this program reserve the right to select for award all, some or none of the proposals submitted in response to this announcement. The DoD agencies provide no funding for direct reimbursement of proposal development costs. Technical and cost proposals (or any other material) submitted in response to this FOA will not be returned. It is the policy of the DoD agencies to treat all proposals as competition sensitive information and to disclose their contents only for the purposes of evaluation.

Please note the following important items:

- Opportunities to attract Australian funding for proposals with Australian collaborators in Topic 1, Topic 5 and Topic 22 are described at http://www.business.gov.au/ausmuri
- There are no topics selected for UK collaboration this year.
- A requirement that the project summary/ abstract required in the submission of the proposal must be publically releasable is noted in Section IV, B, 2.
- The notice that advisors external to the U.S. government may be used as subject-matter-expert technical consultants in the evaluation of the proposals after signing non-disclosure statements is contained in Section V, B.

For grant proposals submitted through Grants.gov, applicants should include responses to the Representations indicated in Section VII. C and D of this FOA and located at http://www.onr.navy.mil/Contracts-Grants/submit-proposal/grants-proposal.aspx

Table of Contents

I.   PROGRAM DESCRIPTION

A.   Agency Name

Office of Naval Research
One Liberty Center
875 North Randolph Street
Arlington, VA 22203-1995

B.   Research Opportunity Title

Fiscal Year (FY) 2018 Department of Defense Multidisciplinary Research Program of the University Research Initiative

C.   Program Name

Multidisciplinary University Research Initiative (MURI)

D.   Research Opportunity Number

N00014-17-S-F006

E.   Response Dates

White Papers: 17 Jul 2017 (Monday) 11:59 PM Eastern Daylight Time

Proposals: 01 Nov 2017 (Wednesday) 11:59 PM Eastern Daylight Time

F.   Research Opportunity Description

The MURI program supports basic research in science and engineering at U.S. institutions of higher education (hereafter referred to as "universities") that is of potential interest to DoD. The program is focused on multidisciplinary research efforts where more than one traditional discipline interacts to provide rapid advances in scientific areas of interest to the DoD. As defined in the DoD Financial Management Regulation:

> Basic research is systematic study directed toward greater knowledge or understanding of the fundamental aspects of phenomena and of observable facts without specific applications towards processes or products in mind. It includes all scientific study and experimentation directed toward increasing fundamental knowledge and understanding in those fields of the physical, engineering, environmental, and life sciences related to long-term national security needs. It is farsighted high payoff research that provides the basis for technological progress (DoD 7000.14-R, vol. 2B, chap. 5, para. 050201.B).

DoD's basic research program invests broadly in many specific fields to ensure that it has early cognizance of new scientific knowledge.

The FY 2018 MURI competition is for the topics listed below.

Detailed descriptions of the topics and the Topic Chief for each can be found in Section VIII, entitled, "SPECIFIC MURI TOPICS," of this FOA. The detailed descriptions are intended to provide the applicant a frame of reference and are not meant to be restrictive to the possible approaches to achieving the goals of the topic and the program. Innovative ideas addressing these research topics are highly encouraged.

White papers and proposals addressing the following topics should be submitted to the Army Research Office (ARO):

Topic 1: Integrated Quantum Sensing and Control for High Fidelity Qubit Operations

Topic 2: Novel solid- state materials and color centers for quantum science and engineering

Topic 3: Controlling Protein Function Using Dynamic Chemical Switches to Modulate Structure

Topic 4: Consolidation of Novel Materials and Macrostructures from a Dusty Plasma

Topic 5: Embodied Learning and Control

Topic 6: Coevolution of Neural, Cognitive, & Social Networks: Mind-Body-Community Connections

Topic 7: Network Games

Topic 8: Modeling Interdependence among Natural Systems and Human Population Dynamics

White papers and proposals addressing the following topics should be submitted to the Air Force Office of Scientific Research (AFOSR):

Topic 9: Physically Viable Learning for Control of Autonomous Dynamical Systems

Topic 10: Nanoscale Vacuum Field Effect Transistors

Topic 11: Molecular-scale Studies of Liquid-Solid Interfaces in Electrochemical Processes

Topic 12: Electromagnetic Non-reciprocity via Temporal Modulation

Topic 13: Heterogeneous Interfaces: Route to New Optoelectronic Properties

Topic 14: Piezoelectric Nanoenergetic Materials with Adaptable and Tailorable Reactivity

Topic 15: Advanced Mean-Field Game Theory for Complex Physical & Socio-Economical Systems

Topic 16: β-Ga2O3 as a High-Critical Field Strength Material for Power Systems

White papers and proposals addressing the following topics should be submitted to the Office of Naval Research (ONR):

Topic 17: Predicting and Validating Pathways for Chemical Synthesis

Topic 18: Synthetic Microbial Electronics

Topic 19: Automated Technical Document Comprehension

Topic 20: Materials for Smart Multifunctional Superstructures [(MS)2]

Topic 21: Advanced Optical Materials that Create Force from Light

Topic 22: In situ Microstructural and Defect Evolution below the Micron Scale in as-Deposited Metal Alloys

Topic 23: Enhancing Thermal Transport at Material Interfaces

Topic 24: Self-Assessment of Proficiency for Autonomous and Intelligent Systems

Proposals from a team of university investigators are warranted when the necessary expertise in addressing the multiple facets of the topics may reside in different universities, or in different departments in the same university. By supporting multidisciplinary teams, the program is complementary to other DoD basic research programs that support university research through single-investigator awards. Proposals shall name one Principal Investigator (PI) as the responsible technical point of contact. Similarly, one institution shall be the primary awardee for the purpose of award execution. The PI shall come from the primary institution. The relationship among participating institutions and their respective roles, as well as the apportionment of funds including sub-awards, if any, shall be described in both the proposal text and the budget.

G. Point(s) of Contact

One or more Research Topic Chiefs are identified for each SPECIFIC MURI TOPIC. Questions of a technical nature on a specific topic shall be directed to one of the Research Topic Chiefs identified in Section VIII entitled "SPECIFIC MURI TOPICS" of this FOA.

Questions of a policy nature for all three (3) services shall be directed to ONR as specified below:

ONR MURI Program Point of Contact:

Dr. Ellen Livingston

MURI Program Manager
Office of Naval Research, Code 03R
Email: ellen.s.livingston@navy.mil

Mailing address:
Office of Naval Research One Liberty Center
875 North Randolph Street, Suite 1409
Arlington, VA 22203-1995

Questions of a business nature for all three (3) services shall be directed to ONR as specified below:

David Broadwell
Grants Officer,
Code 25 Office of Naval Research
875 North Randolph Street
Arlington, VA 22203-1995
Email: david.broadwell@navy.mil

Questions submitted after the Q&A deadline, as noted in the table in Section IV. C. of this FOA, may not be answered. The due date for submission of the white paper and/or proposal will not be extended.

Questions asked that can be answered by a page number in the MURI FOA may not be included in MURI FOA amendment(s). Amendments to this FOA will be generated only if a question is asked that requires the Government to provide information not already contained it the FOA or to clarify FOA language.

FOA amendments, if any, will be posted on the Grants.gov Webpage – http://www.grants.gov/ under the service specific MURI announcement.

H. Instrument Type(s)

It is anticipated that all awards to U.S. institutions resulting from this announcement will take the form of grants. These awards will be governed by the guidance in 2 Code of Federal Regulations (CFR) part 200, "Uniform Administrative Requirements, Cost Principles, and Audit Requirements for Federal Awards," as modified and supplemented by the Department of Defense's (DoD) interim

implementation found at 2 CFR part 1103, "Interim Grants and Cooperative Agreements Implementation of Guidance in 2 CFR part 200" (79 FR 76047, December 19, 2014), all of which are incorporated herein by reference.

Examples of model grants can be found on the ONR website at the following link: http://www.onr.navy.mil/en/contracts-Grants/submit-proposal/grants-proposal/model-grant.aspx

I. Catalog of Federal Domestic Assistance (CFDA) Numbers

12.300   ONR
12.800   AFOSR
12.431   ARO

NOTE: Correct CFDA Number must be used in proposal submission to avoid misrouting.

J. Catalog of Federal Domestic Assistance (CFDA) Titles

Basic and Applied Scientific Research, (ONR)
Air Force Defense Research Sciences Program, (AFOSR)
Basic Scientific Research, (ARO)

II. <u>AWARD INFORMATION</u>

A. Period of Performance

It is anticipated that the awards will be made in the form of grants to universities. The awards will be made at funding levels commensurate with the proposed research and in response to agency missions. Each individual award will be for a three-year base period with one two-year option period to bring the total maximum term of the award to five years. The base and option period, if exercised, will be incrementally funded.

B. Award Amount

The total amount of funding for five years available for grants resulting from this MURI FOA is estimated to be approximately $170 million dollars pending out-year appropriations. MURI awards are contingent on availability of funds, the specific topic, and the scope of the proposed work. Typical annual funding per grant is in the $1.25M to $1.5M range. The amount of the award and the number of supported researchers should generally not exceed the limit specified for the individual topics in Section VIII.

It is strongly recommended that applicants communicate with the Research Topic Chiefs regarding these issues before the submission of formal proposals. Depending on the results of the proposal evaluation, there is no guarantee that any of the proposals submitted in response to a particular topic will be recommended for funding. On the other hand, more than one proposal may be recommended for funding for a particular topic.

III. ELIGIBILITY INFORMATION

A. General Eligibility

This MURI competition is open only to, and proposals are to be submitted only by, U.S. institutions of higher education (universities) including DoD institutions of higher education, with degree-granting programs in science and/or engineering. To the extent that it is a part of a U.S. institution of higher education and is not designated as a Federally Funded Research and Development Center (FFRDC), a University Affiliated Research Center (UARC) or other University Affiliated Laboratory (UAL) is eligible to submit a proposal to this MURI competition and/or receive MURI funds. Ineligible organizations (e.g., industry, DoD laboratories, FFRDCs, and foreign entities) may collaborate on the research but may not receive MURI funds directly or via subaward.

When additional funding for an ineligible organization is necessary to make the proposed collaboration possible, such funds may be identified via a separate proposal from that organization. This supplemental proposal shall be attached to the primary MURI proposal and will be evaluated in accordance with the MURI review criteria by the responsible Research Topic Chief. If approved, the supplemental proposal may be funded using non-MURI or non-Government funds.

IV. APPLICATION AND SUBMISSION INFORMATION

A. Application and Submission Process

Regardless of whether or not a non-MURI funded collaboration is included in the proposal, the same submission process for white papers and proposals will be followed.

The proposal submission process is in two stages. Prospective awardees are encouraged to submit white papers to minimize the labor and cost associated with the production of detailed proposals that have very little chance of being selected for funding. Based on an assessment of the white papers, the responsible Research Topic Chief will provide informal feedback notification to the prospective awardees to encourage or discourage submission of proposals. The Research Topic Chief may also on occasion, provide feedback encouraging re-teaming to strengthen a proposal.

Submission of White Papers: White papers may be submitted via e-mail directly to a Research Topic Chief, via the United States Postal Service (USPS), or via a commercial carrier to the agency specified for the topic. For hard copy submissions, use the addresses provided in Section IV entitled, "Application and Submission Information" paragraph E. "Address for Submission of Hard Copy White Papers." White papers should be stapled in the upper left hand corner; plastic covers or binders should not be used. Separate attachments, such as individual brochures or reprints, will not be accepted. **Do not email 1) .ZIP files; and 2) password protected files.**

White Paper Deadline: The due date and time for receipt of white papers is no later than Monday, 17 Jul 2017, 11:59 P.M. (Eastern Daylight Time).

Evaluation/Notification: Initial evaluations of the white papers will be issued on, or about, Monday, 07 Aug 2017.

Submission of Proposal: Any applicant may submit a proposal even if its white paper was not identified as being of "particular value" to the Government or if no white paper was submitted. However, the initial evaluation of the white papers should give prospective awardee some indication of whether a later proposal would likely result in an award.

<u>Proposal Deadline</u>:   Proposals must be submitted and received electronically through Grants.gov not later than Wednesday, 1 November 2017 at 11:59 PM (Eastern Daylight Time) to be considered for selection. This is the final due date.

You are responsible for making sure your application is submitted, received, and validated by Grants.gov before the application deadline. If you submit your application late, your proposal is ineligible for consideration.

B.   Content and Format of White Papers and Proposals

The white papers and proposals submitted under this FOA are expected to address unclassified basic research. White papers and proposals will be protected from unauthorized disclosure in accordance with applicable laws and DoD regulations.

Applicants are expected to appropriately mark each page of their submission that contains proprietary information.

For proposals containing data that the applicant does not want disclosed to the public for any reason, or used by the Government except for evaluation purposes, the applicant shall mark the title page with the following legend:

"This proposal includes data that shall not be disclosed outside the Government and shall not be duplicated, used, or disclosed--in whole or in part--for any purpose other than to evaluate the proposal or for program coordination. If, however, a grant is awarded to this applicant as a result of-- or in connection with-- the submission of this data, the Government shall have the right to duplicate, use, or disclose the data to the extent provided in the resulting award. This restriction does not limit the Government's right to use information contained in this data if it is obtained from another source without restriction. The data subject to this restriction is contained in (insert numbers or other identification of sheets)."

Also, mark each sheet of data that the applicant wishes to restrict with the following legend: "Use or disclosure of data contained on this sheet is subject to the restriction on the title page of this proposal."

Titles given to the White Papers/Proposals should be descriptive of the basic research they cover and not be merely a copy of the topic title.

<u>Use of Principal Investigator (PI) Over Multiple Proposals/Topics</u>:

     Applicants contemplating the use of an individual as Principal Investigator (PI) for more than one proposal and/or topic are strongly encouraged to contact the Topic Chief(s) prior to white paper submission to determine if the Topic Chief(s) support PI participation in multiple proposals and/or topics. Support of the use of a PI over multiple proposals and/or topics is at the discretion of the Topic Chief(s).

     PI participation in multiple proposals and/or topics shall be identified in all white paper submissions where the PI is proposed. The white paper should also document the amount of time the PI is available for the project(s) and how the PI will manage their time given the possibility of multiple awards.

     Applicants that do not submit white papers, but wish to submit a proposal, shall document PI participation in multiple proposals and/or topics in all proposals where the PI is proposed.

The proposal should also document the amount of time the PI is available for the project(s) and how the PI will manage their time given the possibility of multiple awards.

1. White Papers Submission: Contents and Format of Applications

Each topic in this announcement has one or more Research Topic Chief(s) identified from one of the participating agencies; ONR, AFOSR, or ARO. Prospective applicants shall submit the white paper to one of the Research Topic Chiefs at the agency to which they are applying.

White paper format shall be as follows:

- Paper Size - 8.5 x 11 inch paper
- Margins - 1 inch
- Spacing – single spaced
- Font - Times New Roman, 12 point
- Number of Pages - no more than four (4) single-sided pages (excluding cover letter, cover page, and curriculum vitae). White paper pages beyond the 4-page limit may not be evaluated or read.
- Copies - For Hard Copy Submissions: one (1) original and two (2) copies.

White Paper content shall be as follows:

- A one page cover letter (optional)
- A cover page, labeled "PROPOSAL WHITE PAPER," that includes the FOA number, proposed title, and proposer's technical point of contact, with telephone number, facsimile number, e-mail address, topic number, and topic title
- Identification of the research and issues
- Proposed technical approaches
- Potential impact on DoD capabilities
- Potential team and management plan
- Summary of estimated costs
- Curriculum vitae of key investigators (see Use of Principal Investigator (PI) Over Multiple Proposals/Topics)
- Identification of any Organizational Conflict(s) of Interest (if any) - See Section VII, E. for more details.
- Identification of anticipated human or animal subject research

The white paper should provide sufficient information on the research being proposed (e.g., hypothesis, theories, concepts, approaches, data measurements and analysis, etc.) to allow for an assessment by a technical expert. It is not necessary for white papers to carry official institutional signatures.

2. Proposal Submission through Grants.gov

NOTE: Proposals must be submitted electronically through Grants.gov.

Before you start: Identify the SPECIFIC MURI TOPICS to which you are proposing and obtain the associated agency and Topic Chief for your topic. You will find the topics with the associated agency and Topic Chief listed in Section VIII, entitled "SPECIFIC MURI TOPICS". This information is needed for the grants.gov Agency Routing Identifier and the CFDA number.

Application forms and instructions are available at Grants.gov. To access these materials, go to http://www.grants.gov, and under the Applicants Tab on the main tool bar, select "Apply for Grants". Find registration, login, and search instructions for all users in the Grants.gov Online User Guide.

Follow the instructions in the Grants.gov Online User Guide to get the application package for this MURI FOA.

Content and Form of Application:

Prospective applicants must complete the mandatory forms in accordance with the instructions provided on the forms and the additional instructions below. Files that are attached to the forms must be in Adobe Portable Document Format (PDF) unless otherwise specified in this announcement.

Form: SF 424 (R&R) - Mandatory

Complete all the required fields in accordance with the pop-up instructions on the form. To activate the instructions, turn on the "Help Mode" (icon with the pointer and question mark at the top of the form). The following information must be completed in the SF 424 located on Grants.gov to ensure that the application is directed to the correct individual for review and to be considered for award, Applicants must fill out Block 4 of the SF 424 R&R as follows:

Block 4a "Federal Identifier":
    For ONR, enter N00014;
    For ARO, enter W36QYT;
    For AFOSR, enter FA9550.

Block 4b "Agency Routing Identifier":
    For ONR, Enter the three (3) digit Research Topic Chief's Code and the Research Topic
        Chief's name (last name first) in brackets (e.g., 331 [Smith, John]).
    For ARO, enter the name of the Research Topic Chief.
    For AFOSR, enter the Research Topic Chief's Topic Number (#) and Research Topic
        Chief's name (last name first) in brackets (e.g., 12 [Smith, John]).

Applicants who fail to provide a Research Topic Chief identifier may receive a notice that their proposal is rejected.

Block 4c, "Previous Grants.gov Tracking ID":
    If this submission is for a Changed/ Corrected Application, enter the Grants.gov tracking number of the previous proposal submission; otherwise, leave blank.

Form: RESEARCH & RELATED Other Project Information - Mandatory

Complete all the required fields in accordance with the pop-up instructions on the form.

Field 7: Project Summary/Abstract – Mandatory (Field 7 of the RESEARCH & RELATED Other Project Information)

The project summary/abstract should identify the research problem, technical approaches, anticipated outcome of the research, if successful, and impact on DoD capabilities. It should identify the Principal Investigator; the university and other universities involved in the MURI

team if any; the proposal title; the agency to which the proposal is submitted; and the MURI topic number. Graphics are not allowed and there is a 4,000 character limit including spaces.

The project summary/ abstract must be marked by the applicant as publically releasable.

Abstracts of all funded research projects will be posted on the public DTIC website: https://dodgrantawards.dtic.mil/grants/index.html#/home. Do not include proprietary or confidential information.

For ARO Topics, the Project Summary/Abstract shall be completed on the form entitled "Publicly Releasable Project Abstract" found at the following website: http://www.arl.army.mil/www/default.cfm?page=218.

To attach a Project Summary/Abstract, click "Add Attachment" and attach the project summary/abstract. (Applicants will not be able to type in the box, therefore, save the file to attach as "Project Summary/Abstract").

Field 8 Project Narrative – **Mandatory** (Field 8 of the RESEARCH & RELATED Other Project Information)

To attach a Project Narrative in Field 8 click on "Add Attachment" and attach the technical proposal as a single PDF file. (Save the file as "Volume I- Technical Proposal," as typing in the box is prohibited).

The Following Formatting Rules Apply for Field 8

- Paper size when printed - 8.5 x 11 inch paper
- Margins - 1 inch
- Spacing - single
- Font - Times New Roman, 12 point
- Number of pages in Field 8 - no more than twenty-five (25) single-sided pages.   The cover page, table of contents, list of references, letters of support, curriculum vitae and list of on-going and pending research support are excluded from the page limitations. The pages of proposals exceeding the page limit may not be included in the evaluation.

Include the Following in Field 8

The first page (cover page) of the narrative must include the following information:
- Principal Investigator (PI) name
- Phone number, fax number and e-mail address
- Institution, Department, Division
- Institution address
- Other universities involved in the MURI team
- Is the PI a current DoD Contractor or Grantee?
- If yes, provide Agency, point of contact; and phone number.
- Proposal title
- Institution proposal number
- Agency to which proposal is submitted
- Topic number and topic title

Table of Contents: List project narrative sections and corresponding page numbers.

Technical Approach:

Describe in detail the basic research in science and/or engineering to be undertaken. State the objective and approach, including how data will be analyzed and interpreted. Discuss the relationship of the proposed research to the state-of-the-art knowledge in the field and to related efforts in programs elsewhere, and discuss potential scientific breakthroughs. Include appropriate literature citations/references. Discuss the nature of expected results. Describe plans for the research training of students. Include the number of time equivalent graduate students and undergraduates, if any, to be supported each year. Discuss the involvement of other students, if any.

Project Schedule: A summary of the schedule of events and a detailed description of the expected results.

Management Approach:

• A discussion of the overall approach to the management of this effort, including brief discussions of: required facilities; relationships with any subawardees and with other organizations; availability of personnel; and planning, scheduling and control procedures.

• Describe the facilities available for the accomplishment of the proposed research and related education objectives. Describe any capital equipment planned for acquisition under this program and its application to the proposed research. If possible, budget for capital equipment should be allocated to the first budget period of the grant. Include a description of any government furnished equipment/ hardware/ software/ information, that are required for the proposed effort.

• Describe in detail proposed subawards to other eligible universities or with other eligible institutions. If subawards to other universities are proposed, make clear the division of research activities, to be supported by detailed budgets for the proposed subawards.

• Designate one individual as the Principal Investigator for the award, for the purpose of technical responsibility and to serve as the primary point of contact with an agency's Research Topic Chief. Briefly summarize the qualifications of the Principal Investigator and other key investigators who will conduct the proposed research. Details can be included in the individual CVs.

• Briefly describe the research activities of the Principal Investigator (PI) and co-investigators in on-going and pending research projects, the time charged to each of these projects, and their relationship to the proposed effort. Details should be included in the individual CVs. Provide the percentage of the PI's time which will be allotted to this research project by year and the percentage of his time which is specifically committed or obligated to other activities (e.g. teaching, other grants, contracts, consultancies).

• Describe plans to manage the interactions among members of the proposed research team.

• Identify other parties to whom the proposal has been, or will be sent, including agency contact   information.

List of References: List publications cited in above sections.

Letters of Support: Up to three Letters of Support, describing interest in the topic area or expressing a commitment for support may be included.

Curriculum Vitae: Include curriculum vitae of the Principal Investigator and key co-investigators. List the amount of funding and describe the research activities of the Principal Investigator and key co-investigators in on-going and pending research projects, whether or not acting as Principal Investigator in these other projects.

Field 9: Bibliography & References Cited (Field 9 of the RESEARCH & RELATED Other Project Information)

Field 10: Facilities & Other Resources (Field 10 of the RESEARCH & RELATED Other Project Information)

Field 11: Equipment (Field 11 of the RESEARCH & RELATED Other Project Information)

Field 12: Other Attachments. Budget – Mandatory (Field 12 of the RESEARCH & RELATED Other Project Information)

Attach the budget proposal at Field 12. Prospective applicants must provide a detailed cost breakdown of all costs, by cost category and by the funding periods described below, corresponding to the proposed Technical Approach which was provided in Field 8 of the Research and Related Other Project Information Form.

In addition to attaching the budget proposal at Field 12, the applicant shall also use the Grants.gov forms (including the Standard Form (SF) Research and Related (R&R) Budget Form) from the application package template associated with the FOA on the Grants.gov web site located at: http://www.grants.gov/

The budget shall adhere to the following guidelines.

Detailed breakdown of all costs, by cost category, by the calendar periods stated below. For budget purposes, use an award start date of 01 Jun 2018. For the three-year base grant, the cost should be broken down to reflect funding increment periods of:

(1)   Twelve months,
(2)   Twelve months, and
(3)   Twelve months

Note that the budget for each of the calendar periods should include only those costs to be expended during that calendar period. The budget should also include an option for two additional years broken down to the following funding periods:

(1)   Twelve months, and
(2)   Twelve months

For proposals to ARO topics the Recommended Funding Profile is:

(1)   FY18: Four months (01 Jun 18 to 30 Sep 18): $312,500
(2)   FY19: Twelve months (01 Oct 18 to 30 Sep 19): $1,250,000
(3)   FY20: Twelve months (01 Oct 19 to 30 Sep 20): $1,250,000
(4)   FY21: Eight months (01 Oct 20 to 31 May 21): $937,500

        Three-year base subtotal: $3,750,000

(4)   FY21: Four months (01 Jun 21 to 30 Sep 21): $312,500
(5)   FY22: Twelve months (01 Oct 21 to 30 Sep 22): $1,250,000
(6)   FY23: Eight months (01 Oct 22 to 30 Jun 23): $937,500

        Two-year option subtotal: $2,500,000
        Five-year total: $6,250,000

Annual budget should be driven by program requirements. Elements of the budget should include:

- Direct Labor – Individual labor categories or persons, with associated labor hours and unburdened direct labor rates. Provide any escalation rates for out years.

- Administrative and Clerical Labor – Salaries of administrative and clerical staff are normally indirect costs (and included in an indirect cost rate). Direct charging of these costs may be appropriate when a major project requires an extensive amount of administrative or clerical support significantly greater than normal and routine levels of support. Budgets proposing direct charging of administrative or clerical salaries must be supported with a budget justification which adequately describes the major project and the administrative and/or clerical work to be performed.

- Fringe Benefits and Indirect Costs (F&A, Overhead, G&A, etc.) – The proposal should show the rates and calculation of the costs for each rate category. If the rates have been approved/negotiated by a Government agency, provide a copy of the memorandum/agreement. If the rates have not been approved/ negotiated, provide sufficient detail to enable a determination of allowability, allocability and reasonableness of the allocation bases, and how the rates are calculated. Additional information may be requested, if needed. If composite rates are used, provide the calculations used in deriving the composite rates.

- Travel – The proposed travel cost should include the following for each trip: the purpose of the trip, origin and destination if known, approximate duration, the number of travelers, and the estimated cost per trip must be justified based on the organizations historical average cost per trip or other reasonable basis for estimation. Such estimates and the resultant costs claimed must conform to the applicable Federal cost principals.

- Subawards/Subcontracts – Provide a description of the work to be performed by the subrecipient/ subcontractor. For each subaward, a detailed cost proposal is required to be submitted by the subrecipient(s). A proposal and supporting documentation must be received and reviewed before the Government can complete its cost analysis of the proposal and enter negotiations. The preferred method of receiving subcontract

information is for this information to be included with the Prime's proposal; however, a subcontractor's cost proposal can be provided in a sealed envelope with the recipient's cost proposal or via e-mail directly to the Program Officer at the same time the prime proposal is submitted. The e-mail should identify the proposal title, the prime Applicant, and that the attached proposal is a subcontract. Fee/Profit guidance is noted below.

- Consultants – Provide a breakdown of the consultant's hours, the hourly rate proposed, any other proposed consultant costs, a copy of the signed Consulting Agreement or other documentation supporting the proposed consultant rate/cost, and a copy of the consultant's proposed statement of work, if it is not already separately identified in the prime awardee's proposal.

- Materials & Supplies – Provide an itemized list of all proposed materials and supplies including quantities, unit prices, and the basis for the estimate (e.g., quotes, prior purchases, catalog price lists)

- Recipient Acquired Equipment or Facilities – Equipment and/or facilities are normally furnished by the Recipient. If acquisition of equipment and/or facilities is proposed, a justification for the purchase of the items must be provided. Provide an itemized list of all equipment and/ or facilities costs and the basis for the estimate (e.g., quotes, prior purchases, catalog price lists). Allowable items normally would be limited to research equipment not already available for the project. General purpose equipment (i.e., equipment not used exclusively for research, scientific or other technical activities, such as personal computers, laptops, office equipment) should not be requested unless they will be used primarily or exclusively for the project. For computer/laptop purchases and other general purpose equipment, if proposed, include a statement indicating how each item of equipment will be integrated into the program or used as an integral part of the research effort.

- Other Direct Costs – Provide an itemized list of all remaining proposed other direct costs, such as Graduate Assistant tuition, laboratory fees, report and publication costs, and the basis for the estimate (e.g., quotes, prior purchases, catalog price lists).

- Fee Profit – Fee/profit is unallowable under assistance agreements at either the prime or subaward level but may be permitted on subcontracts issued by the prime awardee.

Form: Project Abstract (Mandatory)

The Project Abstract that is attached here should be the same as the Project Summary/ Abstract attached in Field 7 of the R&R Other Project Information Form.

Submission of Grant Proposals through Grants.gov

Detailed instructions entitled "Grants.Gov Electronic Application and Submission Information" on how to submit a Grant proposal through Grants.gov are under the Acquisition Department - Submitting a Proposal section of the website at http://www.onr.navy.mil/Contracts-Grants/submit-proposal/grants-proposal/grants-gov.aspx

By completing Block 17 of the SF 424 R&R the Grant Applicant is providing the certification on lobbying required by 32 CFR Part 28. Refer to Section VII. OTHER INFORMATION part B, for further information.

For electronic submission of grant proposals, there are several one-time actions that must be completed in order to submit an application through Grants.gov. These include obtaining a Unique Entity Identifier (formerly the Dun and Bradstreet Data Universal Numbering System (DUNS) number), registering with System for Award Management (SAM), registering with the credential provider, and registering with Grants.gov. See www.grants.gov, specifically http://www.grants.gov/web/grants/support.html. Click on Grants.gov Online User Guide.

Use the Grants.gov Organization Registration Checklist which can be found at:

http://www.grants.gov/web/grants/applicants/organization-registration.html

This document will provide guidance through the process. Designating an E-Business Point of Contact (E-Biz POC) and obtaining a special password called 'MPIN' are important steps in the SAM registration process. Applicants who are not registered with SAM.gov and Grants.gov should allow at least 21 days to complete these requirements. The process should be started as soon as possible. Any questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 (1-606-545-5035 for foreign applicants) or support@grants.gov.

Special Notices Relative to Grant Applications to be submitted through Grants.Gov:

All attachments to grant applications submitted through Grants.Gov must be in Adobe Portable Document Format (PDF). Proposals with attachments submitted in word processing, spreadsheet, or any format other than Adobe Portable Document Format (PDF) will not be considered for award.

Proposal Receipt Notices:

After a proposal is submitted through Grants.gov, the Authorized Organization Representative (AOR) will receive a series of three e-mails. It is extremely important that the AOR watch for and save each of the e-mails. Prospective applicants will know that the proposal has reached the DoD agency when the AOR receives E-mail Number 3. Prospective applicants will need the Submission Receipt Number (E-mail Number 1) to track a submission. The three e-mails are:

- E-mail Number 1- The applicant will receive a confirmation page upon completing the submission to Grants.gov. This confirmation page is a record of the time and date stamp that is used to determine whether the proposal was submitted.

- E-mail Number 2 - The applicant will receive an e-mail indicating that the proposal has been validated by Grants.gov within two days of submission (This means that all of the required fields have been completed). After an institution submits an application, Grants.gov generates a submission receipt via email and also sets the application status to "Received." This receipt verifies the Application has been successfully delivered to the Grants.gov system. Next, Grants.gov verifies the submission is valid by ensuring it does not contain viruses, the opportunity is still open, and the applicant login and applicant DUNS number match. If the submission is valid, Grants.gov generates a submission validation receipt via email and sets the application status to "Validated." If the application is not validated, the application status is set to "Rejected." The system sends a rejection email notification to the institution, and the institution must resubmit the application package. Applicants can track the status of their application by logging in to Grants.gov.

- E-mail Number 3 - The third notice is an acknowledgment of receipt in e-mail form from the DoD agency within ten days from the proposal due date, if applicable. The e-mail is sent to the   Authorized Organization Representative (AOR) for the institution. The e-mail for proposals notes that the proposal has been received and provides the assigned tracking number.

C.   Significant Dates and Times

Schedule of Events		
Event	**Date**	**Time**
Questions Regarding white papers*	30 Jun 2017 (Friday)	11:59 PM Eastern Daylight Time
White Papers Due	17 Jul 2017 (Monday)	11:59 PM Eastern Daylight Time
Notification of Initial DoD Evaluations of White Papers	07 Aug 2017 (Monday)**	
Questions Regarding Proposals*	11 Oct 2017 (Wednesday)	11:59 PM Eastern Daylight Time
Proposals Due	01 Nov 2017 (Wednesday)	11:59 PM Eastern Daylight Time
Notification of Selection for Award	30 Mar 2018 (Friday) **	
Start Date of Grant	01 Jun 2018 to 30 Sep 2018 **	

 * Questions submitted after the Q&A deadline as noted in the table above may not be answered. The due date for submission of the white paper and/or proposal will not be extended.

 ** These dates are estimates as of the date of this announcement.

Note: Due to changes in security procedures since September 11, 2001, the time required for hard-copy written materials to be received at any of the DoD Agencies has increased. Materials submitted through the U.S. Postal Service, for example, may take seven days or more to be received, even when sent by Express Mail. Thus, any hard-copy white papers should be submitted in advance of the deadline established in the solicitation so that it will not be received late and thus be ineligible for consideration.

D.   Submission of Late Proposals

The system-generated Grants.gov time stamp is used to determine when you submitted your successfully validated proposal. Grants.gov policies and procedures for application submission and processing apply.

After proposals are uploaded to Grants.gov, the submitter receives an email indicating the proposal has been submitted and that Grants.gov will take up to two days to validate the proposal. As it is possible for Grants.gov to reject the proposal during this process, it is STRONGLY recommended that any proposals be uploaded at least two days before the deadline so that it will not be received late and be ineligible for award consideration. Proposal upload issues with the online Grants.gov system shall be addressed with the Grants.gov Help Desk and not with the DoD agencies.

E.   Address for Submission of Hard Copy White Papers

Submission of white papers shall be sent to the addresses below.

Important Notes Regarding Submission of Hard Copy White Papers: If the Applicant is using USPS, please allow an additional five (5) business days for the package to be delivered due to USPS mail being sent to a central location for special processing before it is sent to the addresses below.

U.S. Army Research Office:
Hard copy white papers addressing topics (1) to (8) should be sent to the U.S. Army Research Office at one of the following addresses:

For delivery by USPS use:
U.S. Army Research Office (FY18 MURI)
P. O. Box 12211
Research Triangle Park, NC 27709-2211

For commercial delivery (such as FedEx, UPS, etc.) use:
U.S. Army Research Office (FY18 MURI)
For white papers include:
ATTN: (list name of responsible Research Topic Chief)
800 Park Office Drive, Suite 4229
Research Triangle Park, NC 27709
919-549-4211

Air Force Office of Scientific Research:
Hard copy white papers addressing topics (9) to (16) should be sent to the Air Force Office of Scientific Research at the following address:

Air Force Office of Scientific Research
ATTN: (list name of responsible Research Topic Chief)
875 North Randolph Street, Suite 325, Room 3112
Arlington, VA 22203-1768
Reference phone # 703-558-1773
Email: chakila.tillie@us.af.mil

Office of Naval Research:
Hard copies of white papers topics (17) to (24) should be sent to the Office of Naval Research at the following address: (For those topics with multiple topic chiefs, send the white paper to the first topic chief listed.)

Primary:
Office of Naval Research
ATTN: (list name of responsible Research Topic Chief)
875 North Randolph Street - Suite W256A*
Arlington, VA 22203-1995
Point of Contact: Paula Barden
Email: paula.barden.ctr@navy.mil
703-696-4111

Secondary:
Office of Naval Research
ATTN: (list name of responsible Research Topic Chief)
875 North Randolph Street - Suite 1409*
Arlington, VA 22203-1995
Point of Contact: Dr. Ellen Livingston
Email: ellen.s.livingston@navy.mil
Phone: 703-696-4668

*This is the address for hand delivery, delivery via USPS and delivery via commercial delivery services. If a telephone number is required, please use 703-696-4111 or 703-696-4668.

V. APPLICATION REVIEW INFORMATION

A. Evaluation Criteria

Basic Research: The MURI Program is funded by a basic research (Budget Activity 1) appropriation. White papers and proposals, in order to be considered for funding, are therefore required to be of a basic, rather than applied or advanced technological, nature.

Note that basic research includes "scientific study and experimentation directed toward increasing fundamental knowledge and understanding" while applied research deals with the development of "useful materials, devices, and systems or methods" and "the design, development, and improvement of prototypes and new processes to meet general mission area requirements." The full definitions of these terms are contained in document: (DoD 7000.14-R, vol. 2B, chap. 5, para. 050201.B)

White papers will be evaluated to assess whether the proposed research is likely to meet the objectives of the specific topic, and thus whether to encourage the submission of a proposal. The assessment of the white papers will primarily focus on scientific and technical merits, potential for the research to significantly advance fundamental understanding in the topic area, and potential DoD interest.

Proposals responding to this FOA in each topic area will be evaluated using the following criteria:

- Scientific and technical merits of the proposed basic science and/or engineering research;
- Potential for the research, if successful, to significantly advance fundamental understanding in the topic area;
- DoD potential interest in the proposed research;
- Qualifications and availability of the Principal Investigator and other investigators;
- Adequacy of current or planned facilities and equipment to accomplish the research objectives;
- Impact of interactions with other organizations engaged in related research and development, in particular DoD laboratories, industry, and other organizations that perform research and development for defense applications; and
- Realism and reasonableness of cost (cost sharing is not a factor in the evaluation)

The Government will evaluate options for award purposes by adding the total cost for all options to the total cost for the basic requirement. Evaluation of options will not obligate the Government to exercise the options during grant performance.

B. Evaluation Panel

White paper submissions will be reviewed either solely by the responsible Research Topic Chief for the specific topic or by an evaluation panel chaired by the responsible Research Topic Chief. An evaluation panel will consist of technical experts who are Government employees or who are

detailed under the Intergovernmental Personnel Act (IPA). Restrictive notices notwithstanding, one or more support contractors or advisors external to the US Government may be utilized as subject-matter-expert technical consultants. These individuals will sign a conflict of interest statement and a non-disclosure agreement prior to receiving proposal information.

Proposals will undergo a multi-stage evaluation procedure. The Research Topic Chief and other Government scientific experts will perform the evaluation of technical proposals first. Cost proposals will be evaluated by Government business professionals. Restrictive notices notwithstanding, one or more support contractors or advisors external to the US Government may be utilized as subject-matter-expert technical consultants. However, proposal selection and award decisions are solely the responsibility of Government personnel. Support contractor employees and advisors external to the US Government having access to technical and cost proposals submitted in response to this FOA will be required to sign a non-disclosure and a conflict of interest statement prior to receipt of any proposal submission. Findings of the evaluation panels will be forwarded to senior DoD officials who will make funding recommendations to the awarding officials.

Due to the nature of the MURI program, the evaluation panels and reviewing officials may on occasion recommend that less than an entire MURI proposal be selected for funding. This may be due to several causes, such as insufficient funds, research overlap among proposals received, or potential synergies among proposals under a research topic. In such cases, proposal adjustments will be agreed to by the Principal Investigator and the Government prior to final award.

C. General Information Regarding the Review and Selection Process for Grants

1) Prior to making an award with total amount of Federal share greater than the simplified acquisition threshold, the Grant Officer shall review and consider any information about the applicant that is in the designated integrity and performance system accessible through the System for Award Management (SAM) (currently Federal Awardee Performance and Integrity System, FAPIIS).

2) The applicant, at its option, may review information in the designated integrity and performance systems accessible through SAM and comment on any information about itself that a Federal awarding agency previously entered and is currently in the designated integrity and performance system accessible through SAM.

3) The Grant Officer will consider any comments by the applicant, in addition to the other information in the designated integrity and performance system, in making a judgment about the applicant's integrity, business ethics, and record of performance under Federal awards when completing the review of risk posed by the applicant as described in Title 2, Part 200, Subsection 200.205 Federal awarding agency review of risk posed by applicants.

VI. AWARD ADMINISTRATION INFORMATION

A. Administrative Requirements

System for Award Management (SAM): All Applicants submitting proposals must:

1) Be registered in the SAM prior to submission;
2) Maintain an active SAM registration with current information at all times during which it has an active Federal award or an application under consideration by any agency; and
3) Provide its DUNS number in each application or proposal submitted to the agency.

SAM may be accessed at https://www.sam.gov/portal/public/SAM/

B. Reporting

In general, for each grant award, annual reports and a final report are required to summarize the technical progress and accomplishments during the performance period, as well as any other report requested by the Research Topic Chief.

C. Access to your Award

ARO: ARO emails their awards/ modification documents to the awardees.

AFOSR: AFOSR emails their awards/ modification documents to the awardees.

ONR: ONR award/ modification documents are only available via the Department of Defense (DoD) Electronic Document Access System (EDA) within the Wide Area WorkFlow e-Business Suite (https://wawf.eb.mil/).

> EDA is a Web-based system that provides secure online access, storage and retrieval of awards and modifications to DoD employees and vendors. ONR creates an award notification profile for every award. For grants, the notification profile will use the email addresses from the Application for Federal Assistance, SF424, to notify the recipient of an award. ONR is using the following three email addresses entered by the grantee on the SF424 application to create the EDA notification profile:

> a. Applicant Information (Block 5 - Email)
> b Project Director / Principal Investigator (Block 14 - Email)
> c. Authorized Representative (Block 19 - Email)

> *IMPORTANT*: In some cases, EDA notifications are appearing in recipients' Junk Email folder. If you are experiencing issues receiving EDA notifications, please check your junk email. If found, please mark EDA notifications as "not junk."

> If you do not currently have access to EDA, you may complete a self-registration request as a "Vendor" via https://wawf.eb.mil/ following the steps below:

> Registration questions may be directed to the EDA help desk toll free at 866-618-5988, commercial at 801-605-7095, or via email at disa.ogden.esd.mbx.cscassig@mail.mil

VII. OTHER INFORMATION

A. Federal Funding Accountability and Transparency Act of 2006 –

The Federal Funding Accountability and Transparency Act of 2006 (Public Law 109-282), as amended by Section 6202 of Public Law 110-252, requires that all agencies establish requirements for recipients reporting information on subawards and executive total compensation as codified in 2 CFR Part 170. Any company, non-profit agency or university that applies for financial assistance as either a prime or sub-recipient under this FOA must provide information in its proposal that describes the necessary processes and systems in place to comply with the reporting requirements identified in 2 CFR Part 170 Appendix A. Entities are required to meet reporting requirements unless an exception or exemption applies. Refer to 2 CFR Part 170, including Appendix A, for a detailed explanation of the requirements, exceptions, and exemptions.

B. Certification regarding Restrictions on Lobbying –

Grant and Cooperative Agreement awards greater than $100,000, as well as OTAs not under Section 845, require a certification of compliance with a national policy mandate concerning lobbying. Grant applicants shall provide this certification by electronic submission of SF424 (R&R) as a part of the electronic proposal submitted via Grants.gov (complete Block 17).   The following certification applies likewise to each Cooperative Agreement and normal OTA applicant seeking federal assistance funds exceeding $100,000:

(1) No Federal appropriated funds have been paid or will be paid by or on behalf of the applicant, to any person for influencing or attempting to influence an officer or employee of an agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any Federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.

(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the Federal contract, grant, loan, or cooperative agreement, the applicant shall complete and submit Standard Form-LLL, "Disclosure Form to Report Lobbying," in accordance with its instructions.

(3) The applicant shall require that the language of this certification be included in the award documents for all subawards at all tiers (including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements) and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by Section 1352, title 31, U.S.C.
Any person who fails to file the required certification shall be subject to a civil penalty of not less than $10,000 and not more than $100,000 for each such failure.

C. Representation Regarding an Unpaid Delinquent Tax Liability or a Felony Conviction Under any Federal Law - DoD Appropriations –

All grant applicants are required to complete the "Representation on Tax Delinquency and Felony Conviction" found at http://www.onr.navy.mil/Contracts-Grants/submit- proposal/grants-proposal.aspx by checking the "I agree" box in block 17 and attaching the representation to block 18 of the SF424 (R&R) as part of the electronic proposal submitted via Grants.gov. The representation reads as follows:

(1) The applicant represents that it _____ is not _____ a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.

(2) The applicant represents that it _____ is not _____ a corporation that was convicted of a felony criminal violation under any Federal law within the preceding 24 months. NOTE: If an applicant responds in the affirmative to either of the above representations, the applicant is ineligible to receive an award unless the agency suspension and debarment official (SDO) has considered suspension or debarment and determined that further action is not required to protect the Government's interests. The applicant therefore must provide information about its tax liability or conviction to the agency's SDO as soon as it can do so, to facilitate completion of the required consideration before award decisions are made.

D. Representation Regarding the Prohibition on Using Funds with Entities that Require Certain Internal Confidentiality Agreements –

Agreement with the representation below will be affirmed by checking the "I agree" box in block 17 of the SF424 (R&R) as part of the electronic proposal submitted via Grants.gov. The representation reads as follows:

By submission of its proposal or application, the applicant represents that it does not require any of its employees, contractors, or subrecipients seeking to report fraud, waste, or abuse to sign or comply with internal confidentiality agreements or statements prohibiting or otherwise restricting those employees, contractors, subrecipients from lawfully reporting that waste, fraud, or abuse to a designated investigative or law enforcement representative of a Federal department or agency authorized to receive such information.

Note that, as applicable, the bases for this representation are the prohibition(s) as follow:

    i.   Section 743 of the Financial Services and General Government Appropriation Act, 2015 (Division E of the Consolidated and Further Continuing Appropriations Act, 2015, Pub. L. 113-235).

    ii.   Section 101(a) of the Continuing Appropriation Act, 2016 (Pub. L. 114-53) and any subsequent FY2016 appropriations act that extends to FY2016 the same restrictions as are contained in section 743 of Division E, title VII of the Consolidated and Further Continuing Appropriations Act, 2015 (Pub L. 113-235).

    iii.   Pub. L. 114-223, Continuing Appropriations Act, 2017, or any other Act that extends to fiscal year 2017 funds the same prohibitions as contained in section 743, Division E, title VII, of the Consolidated Appropriations Act, 2016 (Pub. L. 114-113).

    iv.   Any successor provision of law on making funds available through grants and cooperative agreements to entities with certain internal confidentiality agreements or statements.

The prohibitions stated above do not contravene requirements applicable to Standard Form 312, Form 4414, or any other form issued by a Federal department or agency governing the nondisclosure of

classified information.

E. Code of Conduct –

Applicants for grants, cooperative agreements, or other transaction agreements as applicable are required to comply with 2 CFR 200.318(c), Codes of Conduct, to prevent real or apparent conflicts of interest in the award and administration of any contracts supported by federal funds. This provision will be incorporated into all assistance instruments awarded under this FOA.

F. Reporting –

If the Federal share of any Federal award may include more than $500,000 over the period of performance, the post award reporting requirements , Award Term and Condition for Recipient Integrity and Performance Matters (2 U.S.C. 200 Appendix XII), is applicable as follows:

    1. Reporting of Matters Related to Recipient Integrity and Performance

        a. General Reporting Requirement

        If the total value of your currently active grants, cooperative agreements, and procurement contracts from all Federal awarding agencies exceeds $10,000,000 for any period of time during the period of performance of this Federal award, then you as the recipient during that period of time must maintain the currency of information reported to the System for Award Management (SAM) that is made available in the designated integrity and performance system (currently the Federal Awardee Performance and Integrity Information System (FAPIIS)) about civil, criminal, or administrative proceedings described in paragraph 2 of this award term and condition. This is a statutory requirement under section 872 of Public Law 110-417, as amended (41 U.S.C. 2313). As required by section 3010 of Public Law 111-212, all information posted in the designated integrity and performance system on or after April 15, 2011, except past performance reviews required for Federal procurement contracts, will be publicly available.

    2. Proceedings About Which You Must Report

    Submit the information required about each proceeding that:

        a. Is in connection with the award or performance of a grant, cooperative agreement, or procurement contract from the Federal Government;

        b. Reached its final disposition during the most recent five year period; and

        c. Is one of the following:

            (1) A criminal proceeding that resulted in a conviction, as defined in paragraph 5 of this award term and condition;

(2) A civil proceeding that resulted in a finding of fault and liability and payment of a monetary fine, penalty, reimbursement, restitution, or damages of $5,000 or more;

(3) An administrative proceeding, as defined in paragraph 5. of this award term and condition, that resulted in a finding of fault and liability and your payment of either a monetary fine or penalty of $5,000 or more or reimbursement, restitution, or damages in excess of $100,000; or

(4) Any other criminal, civil, or administrative proceeding if:

(i) It could have led to an outcome described in paragraph 2.c.(1), (2), or (3) of this award term and condition;

(ii) It had a different disposition arrived at by consent or compromise with an acknowledgment of fault on your part; and

(iii) The requirement in this award term and condition to disclose information about the proceeding does not conflict with applicable laws and regulations.

3. Reporting Procedures

Enter in the SAM Entity Management area the information that SAM requires about each proceeding described in paragraph 2 of this award term and condition. You do not need to submit the information a second time under assistance awards that you received if you already provided the information through SAM because you were required to do so under Federal procurement contracts that you were awarded.

4. Reporting Frequency

During any period of time when you are subject to the requirement in paragraph 1 of this award term and condition, you must report proceedings information through SAM for the most recent five year period, either to report new information about any proceeding(s) that you have not reported previously or affirm that there is no new information to report. Recipients that have Federal contract, grant, and cooperative agreement awards with a cumulative total value greater than $10,000,000 must disclose semiannually any information about the criminal, civil, and administrative proceedings.

5. Definitions

For purposes of this award term and condition:

a. Administrative proceeding means a non-judicial process that is adjudicatory in nature in order to make a determination of fault or liability (e.g., Securities and Exchange Commission Administrative proceedings, Civilian Board of Contract Appeals

proceedings, and Armed Services Board of Contract Appeals proceedings). This includes proceedings at the Federal and State level but only in connection with performance of a Federal contract or grant. It does not include audits, site visits, corrective plans, or inspection of deliverables.

b. Conviction, for purposes of this award term and condition, means a judgment or conviction of a criminal offense by any court of competent jurisdiction, whether entered upon a verdict or a plea, and includes a conviction entered upon a plea of nolo contendere.

c. Total value of currently active grants, cooperative agreements, and procurement contracts includes—

(1) Only the Federal share of the funding under any Federal award with a recipient cost share or match; and

(2) The value of all expected funding increments under a Federal award and options, even if not yet exercised.

G. Requirements Concerning Live Organisms:

1. Use of Animals:

If animals are to be utilized in the research effort proposed, the Applicant must submit a Full Appendix or Abbreviated Appendix with supporting documentation (copies of IACUC Approval, IACUC Approved Protocol, and most recent USDA Inspection Report) prior to award. For assistance with submission of animal research related documentation, contact the ONR Animal Use Administrator at (703) 696-4046. Guidance: http://www.onr.navy.mil/en/About-ONR/compliance-protections/Research-Protections/Animal-Recombinant-DNA.aspx

2. Use of Human Subjects in Research:

a. You must protect the rights and welfare of individuals who participate as human subjects in research under this award and comply with the requirements of the Common Rule at 32 CFR part 219 and applicable provisions of DoD Instruction 3216.02, Protection of Human Subjects and Adherence to Ethical Standards in DoD-Supported Research (2011), the DON implementation of the human research protection program contained in SECNAVINST 3900.39D (or its replacement), 10 USC 980 "Limitation on Use of Humans as Experimental Subjects," and when applicable, Food and Drug Administration (FDA) and other federal and state law and regulations.

b. For proposals containing activities that include or may include "research involving human subjects" as defined in DoDI 3216.02, prior to award, the Applicant must submit documentation of:

(i) Approval from an Institutional Review Board (IRB) (IRB-approved research protocol, IRB- approved informed consent document, and other material they considered); proof of completed human research training (e.g., training certificate or institutional verification of training for the principal investigator, co-investigators); and the Applicant's Department of Health and Human Services (DHHS)-issued Federalwide Assurance (FWA#),

(ii) Any claimed exemption under 32 CFR 219 101(b), including the category of exemption, supporting documentation considered by your institution in making the determination (e.g., protocol, data collection tools, advertisements, etc.). The documentation shall include a short rationale supporting the exemption determination. This documentation should be signed by the IRB Chair or IRB vice Chair, designated IRB administrator or official of the human research protection program.

(iii) Any determinations that the proposal does not contain activities that constitute research involving human subjects, including supporting documentation considered by your institution in making the determination. This documentation should be issued by the IRB Chair or IRB vice Chair, designated IRB administrator or official of the human research protection program.

(c) Documentation must be submitted to the ONR Human Research Protection Official (HRPO), by way of the ONR Program Officer. If the research is determined by the IRB to be greater than minimal risk, you also must provide the name and contact information for the independent research monitor and a written summary of the monitors' duties, authorities, and responsibilities as approved by the IRB. For assistance with submission of human subject research related documentation, contact the ONR Human Research Protection Official (HRPO) at (703) 696-4046.

(d) Research involving human subjects must not be commenced under any award or modification or any subcontract or grant subaward or modification until awardee receives notification from the Grants Officer that the HRPO has approved the assurance as appropriate for the research under the award or modification and that the HRPO has reviewed the protocol and accepted the IRB approval or determination for compliance with Federal, DoD and DON research protection requirements. See, DFARS 252.235-7004. Guidance: http://www.onr.navy.mil/About-ONR/compliance-protections/Research-Protections/Human-Subject-Research.aspx

3. Use of Recombinant DNA or Synthetic Nucleic Acid Molecules:

    Proposals which call for experiments using recombinant or synthetic nucleic acid molecules must include documentation of compliance with NIH Guidelines for Research Involving Recombinant or Synthetic Nucleic Acid Molecules (NIH Guidelines), approval of the Institutional Biosafety Committee (IBC), and copies of the DHHS Approval of the IBC

letter. Guidance: http://www.onr.navy.mil/About-ONR/compliance-protections/Research-Protections/Animal-Recombinant-DNA.aspx

H. Institutional Dual Use Research of Concern:

As of September 24, 2015, all institutions and United States Government (USG) funding agencies subject to the United States Government Policy for Institutional Oversight of Life Sciences Dual Use Research of Concern must comply with all the requirements listed therein. If your research proposal directly involves certain biological agents or toxins, contact the cognizant Technical Point of Contact.. U.S. Government Science, Safety, Security (S3) guidance may be found at http://www.phe.gov/s3/dualuse.

I. Department of Defense High Performance Computing Program:

The DoD High Performance Computing Program (HPCMP) furnishes the DoD S&T and RDT&E communities with use-access to very powerful high performance computing systems. Awardees of ONR contracts, grants, and other assistance instruments may be eligible to use HPCMP assets in support of their funded activities if ONR Program Officer approval is obtained and if security/screening requirements are favorably completed. Additional information and an application may be found at http://www.hpcmo.hpc.mil/.

J. Project Meetings and Reviews –

Individual program reviews between the sponsor and the performer may be held as necessary. Program status reviews may also be held to provide a forum for reviews of the latest results from experiments and any other incremental progress towards the major demonstrations. These meetings will be held at various sites throughout the country. For costing purposes, applicants must assume that 40% of these meetings will be at or near the government sponsor location and 60% at other contractor or government facilities. Interim meetings are likely, but these will be accomplished via video telephone conferences, telephone conferences, or via web-based collaboration tools.

VIII. SPECIFIC MURI TOPICS

ARO

Topic 1: Integrated Quantum Sensing and Control for High Fidelity Qubit Operations

Topic 2: Novel solid- state materials and color centers for quantum science and engineering

Topic 3: Controlling Protein Function Using Dynamic Chemical Switches to Modulate Structure

Topic 4: Consolidation of Novel Materials and Macrostructures from a Dusty Plasma

Topic 5: Embodied Learning and Control

Topic 6: Coevolution of Neural, Cognitive, & Social Networks: Mind-Body-Community Connections

Topic 7: Network Games

Topic 8: Modeling Interdependence among Natural Systems and Human Population Dynamics

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ONR

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Topic 23: Enhancing Thermal Transport at Material Interfaces

Topic 24: Self-Assessment of Proficiency for Autonomous and Intelligent Systems

Topic 1 (ARO): Integrated Quantum Sensing and Control for High Fidelity Qubit Operations

Background: A multidisciplinary focus on qubit physics, materials, fabrication, and operation has resulted in orders of magnitude improvements in key qubit performance metrics. Concurrently, new computer science, statistics, and engineering based control techniques such as Hamiltonian parameter estimation, machine learning, and robust control of classical fields have enabled novel quantum control and feedback approaches. The time is opportune to expand the necessary multidisciplinary approach to a systems view of a complex quantum system operating in a classical environment by integrating the new control, feedback, and sensing concepts with qubit physics to provide the next order of magnitude improvement in qubit performance. Currently, in state-of-the-art, the qubit classical environment is rarely fully characterized during qubit operations in a qubit focused, rather than an integrated system focused, experiment. Potential environmental decohering factors include uncontrolled optical, microwave, and magnetic fields; bias voltages and currents; temperature; and pressure. Qubits often provide the most sensitive and precise measurements of the variability and noise in the classical environment in which they operate and, consequently, have recently been developed as high-performance sensing and metrology tools. These recent quantum sensing advances provide the opportunity for real-time control of the qubit classical environment via a novel combination of qubit sensing, statistics, machine learning, and control approaches. In the new paradigm, qubit sensor based characterization and verification of classical control fields conducted by a distinct set of "spectator" qubits located in the vicinity of the data qubits is visualized. Data qubits concurrently carry out the target quantum operations and operate in the same classical environment as the spectator qubits. In this parallel scheme spectator qubit measurements are inputs in advanced dynamic "closed" loop feedback control strategies that result in fully characterized, verified, and controlled classical environment fields, thereby enabling the realization of very high fidelity data qubit operations.

Objectives: The objectives of the topic are to (i) discover and devise approaches in which new, sensing, "spectator" qubits enable real-time characterization and verification of classical environmental factors which, when uncontrolled, decohere qubits; (ii) develop optimal statistics and computer science based techniques for collecting and analyzing spectator qubit data; and (iii) formulate novel spectator qubit based feedback and control paradigms and advance a new research area in quantum control.

Research Concentration Areas: Work should advantageously leverage recent progress in quantum sensing and measurement, statistics, and machine learning to develop and advance novel control techniques to achieve the objectives. Research should focus on the foundations and development of the "spectator" qubit control concept along with experimental demonstrations of feasibility. Research concentration areas might include: (1) optimal integration of spectator qubits into multi-qubit systems including qubit type, physical layout, initialization, manipulation, and measurement; (2) development of novel statistical, machine learning, and similar approaches for collecting and analyzing spectator qubit data to fully characterize and verify the classical environment; (3) exploration of robust control of statistical properties of classical fields in the regime of sparse measurements as well as learning control protocols for uncertain systems to advance very high fidelity qubit operations.

Anticipated Resources: Awards under this topic will be no more than $1.25M per year for five years, supporting no more than 6 principal and co-principal investigators. Team members should include physicists, statisticians and/or mathematicians, computer scientists, and control theory experts.

- For Topic 1, proposals are invited that include participation from Australian (AU) academic institutions; however, AU participation is not a requirement. In the case of proposals with AU participation, there still should be a single US primary institution and one PI submitting the overall proposal. Funding for the AU participation will be allocated separately by the AU government. Opportunities for Australian funding for such collaborative proposals are described at http://www.business.gov.au/ausmuri

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Topic 2 (ARO): Novel solid- state materials and color centers for quantum science and engineering

Background: Although significant progress has been achieved in understanding and utilizing the quantum properties of optically addressable nitrogen-vacancy (N-V) color centers in diamond for quantum sensing, communication etc., further advances are severely limited by difficulties in achieving exact placement of N-V centers, light collection due to the high refractive index of diamond, large scale integration, and low qubit yield. Superior solid-state host materials such as 3D wide bandgap (WBG) semiconductors (e.g. SiC, ZnO etc.) and recently discovered atomically thin two dimensional (2D) van der Waals materials (e.g. h-BN, WSe_2 etc.) with varieties of optically addressable color centers (far beyond N-V centers) are very attractive alternatives to advance this science. In addition, these alternative materials could also offer new opportunities not yet accessible such as multi-photon states, interactions between color centers and non-linear quantum optics etc. WBG materials offer varieties of color centers with narrow tunable spectral emissions as well as allow integration with nano-photonics etc. possible. With the advent of novel 2D materials, the control of different color centers (placement/density) with atomic precision (e.g. using a scanning tunneling microscope) now appears to be within reach. Furthermore, these flexible 2D materials offer a unique capability to tune optical transitions using strain which was not previously possible with diamonds. Hybrids of 2D materials and WBG materials or 2D hetero-structures (stacks of dissimilar 2D materials) with different color centers could also allow multifunctional sensing. However, the synthesis of isotope free quantum grade novel host materials, identification and incorporation of unique color centers, characterization of their quantum properties (coherence times, spectral stability etc.) and the understanding of their interactions with the external excitations (optical, electrical etc.) still remain significant challenges/unknowns.

Objectives: To develop novel solid state host materials with unique color centers exhibiting extraordinary quantum properties at room temperature (low spectral diffusion, long coherence times etc.), determine the composition- processing- defect- property relationships governing these unique properties, and explore new concepts in quantum science (e.g. multi-photon states etc.) enabled by these new materials.

Research Concentration Areas: Suggested research concentration areas include but are not limited to 1) Design and synthesize selective quantum grade quality novel host materials (WBG materials e.g. ZnO, Ga_2O_3, AlN etc., 2D materials e.g. h-BN, WSe_2 etc., hetero-structures, hybrids) with desired color centers exhibiting unique quantum properties 2) Elucidate the physical mechanisms responsible for the observed novel quantum properties (e.g. spin coherence) and governing composition- processing-defect- property relationships 3) Develop unique characterization techniques tailored to varieties of excitations (optical/electrical/magnetic/thermal/strain etc.) and sensing techniques 4) Employ theory and integrated modeling/simulations to guide experimental efforts and explore new quantum science opportunities such as collective states that could be enabled by the novel color centers/host materials 5) Explore innovative device designs (sensors, quantum repeaters etc.) based on novel qubits.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an average of $1.25M per year for 5 years, supporting no more than 7 funded faculty researchers.

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Topic 3. (ARO): Controlling Protein Function Using Dynamic Chemical Switches to Modulate Structure

Background: In biological systems, function is determined by structure. This structure-function relationship is particularly striking for proteins, where function is not solely determined by a static structure, but is also dependent on dynamic motions of subdomains within the folded protein. The most commonly observed domain motions are hinge and shear motions that occur in response to ligand binding, such as the hinge closure of hexokinase upon binding of glucose. To realize the full promise of engineered biological systems, mechanisms to exert dynamic control over protein structure are critical to enable regulation of protein activity. In recent years, a variety of dynamic bonding schemes have been introduced into synthetic polymer systems that enable triggered structural changes in response to applied stimuli, such as light, changes in pH, mechanical stress, and redox conditions. In these structurally dynamic polymers, macroscopic changes originate from a change in the polymer's molecular architecture through the controlled formation/breakage of bonds, providing a linkage between molecular structure and macroscopic properties that is not typically inherent in synthetic polymer systems. These dynamic chemical switches provide an opportunity to bring structural, and thus functional, control to protein biopolymers.

Chemists have recently demonstrated incorporation of non-natural chemical functional groups into proteins that support synthetic bonding chemistries, including novel protecting groups that provide control over the accessibility of bonding moieties using applied external stimuli. Moreover, as mentioned above, a variety of dynamic chemical switches have been developed for synthetic polymer systems in recent years, expanding the range of dynamic bonding chemistries that could be used for protein engineering. In addition, improved bioinformatics platforms and computational modeling approaches focused on protein structure prediction based on sequence have recently been demonstrated and provide an avenue to guide design of proteins in which engineered activities are linked to directed structural motions. These complementary advances provide an opportunity to explore novel dynamic bonding chemistries as an approach to control the activity of proteins via triggered structural modulation of protein domains, which would significantly expand the design space available for engineered biological and hybrid biotic-abiotic systems and would also have implications for foldable non-biological polymers.

Objective: The objective of this MURI is to enable dynamic control over the motion of protein domains via incorporation of stimuli-responsive dynamic bonding chemistries (excluding disulfide/thiol linkages) to control protein function.

Research Concentration Areas: Suggested research areas include, but are not limited to:
1) Develop reaction schemes for dynamic chemical switches that are compatible with solution conditions required for protein stability and activity. **2)** Develop predictive computational models that incorporate dynamic non-natural bonds into protein structures. **3)** Develop approaches to analyze protein conformation with enhanced resolution in space and time. **4)** Develop approaches to introduce reactive groups into protein chains that will form dynamic bonds (e.g., non-natural amino acids) to provide handles for stimuli-responsive structural conformation changes. **5)** Develop approaches to experimentally validate designed protein motions and to characterize predicted function.

Anticipated Resources: $1.25M/year for 5 years to support up to six funded faculty members.

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<u>Topic 4 (ARO): Consolidation of Novel Materials and Macrostructures from a Dusty Plasma</u>

Background: Research over the last decade has demonstrated that plasmas offer a means of levitating and manipulating "dust" particles of any material into controlled organized structures (i.e., plasma "crystals") of up to tens of cm in size. Concurrently, magnetic plasma confinement chambers have shown abundant material accumulation and fast convective transport. This accumulation motivated advances in the understanding of plasma magnetohydrodynamics (MHD), in addition to accurate predictions of the spatial distribution of dust particles and their individual trajectories. These efforts provide the scientific basis to realize a new paradigm in custom material design: consolidation of 3D free-standing materials and structures from plasma "dust". Plasma-based consolidation could enable unprecedented arrangements of dissimilar particles, phases, and compositions. As plasmas can be created from any element and any material can be arranged in a plasma crystal, novel chemical reactions can be identified incorporating the free electrons, ions, and neutrals of a plasma to enhance manipulation and consolidation. The application of devitrification and agglomeration theories to plasma crystals may also enable the creation of new kinetically stabilized materials. Plasma-based powder synthesis has already created unique morphologies, phases, and control. A robust plasma consolidation process can enable the fabrication of unique composites and shapes that cannot be conventionally machined. While the energy and control required to consolidate a plasma directly would be impractical, the solid dust particles in dusty plasmas can be manipulated with multiple degrees of freedom, provided by electric and magnetic fields, into controlled assemblies via electrostatic forces and MHD. Subsequent complementary consolidation and/or densification could be achieved by methods such as solid or liquid state sintering via heat and/or pressure, flash sintering via directed electrical currents, self-propagating high temperature synthesis, and circulating convection processing.

Objective: The objective is to elucidate and control plasma-material dynamics, concomitant with complementary novel consolidation strategies, in order to realize robust plasma-based synthesis of 3-dimensional free standing macrostructures via controlled consolidation of a wide range of discrete dust particles. Structures fabricated in this manner should be of sufficient size and mechanical strength to be handled directly.

Research Concentration Areas: Suggested research areas include, but are not limited to: 1. *In-situ characterization of plasma/material interactions*: enhancement or development of spectroscopic and other applicable characterization methods for direct observation of plasma/material interactions and the dynamics of the consolidation process. *2. Integrated computational – experimental analysis of dust particle motion and trajectory:* prediction of the motion and distribution of dust particles in response to electrostatic and MHD forces to facilitate validation with experimental measurements, and development of optimized control strategies for dust particle manipulation and consolidation. *3. Development of novel manipulation and consolidation processes:* refine or modify plasma and materials processing tools to achieve bulk manipulation and scalable consolidation of first-of-their-kind 3D macrostructures.

Anticipated Resources: It is anticipated that awards under this topic will be no more than $1.25M per year for 5 years, supporting no more than 5 funded faculty researchers.

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Topic 5 (ARO): Embodied Learning and Control

Background: Progress in agile robotics is currently limited by control methods reliant on optimization about linearized passive dynamics and nearly ideal sensing. In addition, due to the inability of state-of-the-art deep learning methods to handle time-varying data, learning is often only attempted in static environments. As a result, synthetic systems exhibit crippling fragility in unstructured and rapidly changing environments. In biology, this problem is diversely addressed through morphologies supporting hierarchical information processing augmented by strong coupling between highly distributed sensing and actuation, material properties, and physical dynamics. For example, perception in neuromuscular systems is augmented by integrating learned motor patterns, proprioception driven neural reflexes, and mechanical preflexes to achieve robust adaptive locomotion. Thus, embodied learning and control concerns fundamental understanding of processes underlying how natural and artificial systems, independent of particular morphologies, learn to exploit latent dynamics through distributed sensing and actuation to enable rapid transitions from reinforcement learning to model-predictive or anticipatory modes. Four major transdisciplinary advances suggest potential for achieving this goal: (1) morphological computing research has uncovered hidden computational advantages of nonlinearity and mechanical memory in soft systems, (2) robotic materials research has linked amorphous computing with distributed actuation and control in flexible substrates; (3) physics of information research has shown how a system's dynamics becomes an implicit model of environmental fluctuations—linking effective use of information and memory with thermodynamic dissipation; and (4) by leveraging (3), control theorists recently demonstrated rapid learning in nonlinear systems operating in austere environments by exploiting information-theoretic interpretations of energetic concepts in statistical physics.

Objective: Explore the emergence of embodied learning and control within natural and synthetic systems operating in uncertain and changing environments to develop a methodology that predicts statistical synchronization patterns between intrinsic nonlinear dynamics, sensing, and actuation to enable real-time model learning and adaptation.

Research Concentration Areas: Suggested research concentrations include, but are not limited to: (1) novel statistical learning methods for sparse time-varying data (e.g. reservoir computing) with fundamental understanding of the mathematical structures and information thermodynamic mechanisms underlying the algorithms; (2) formalisms for mechanical information processing in dynamical systems exhibiting nonlinearity, memory, and potentially infinite dimensionality with a framework for understanding how to embed, error-correct, and extract high-dimensional information through a limited number of mechanical degrees of freedom; (3) active control of highly distributed sensing and actuation to enable optimal non-equilibrium environmental energetic and information transfer to generate predictive models; (4) understanding tradeoffs between mathematical representations of uncertainty and decision time scales to enable real-time model inference, reinforcement learning, model-predictive control; and (5) thermodynamically efficient methods for actively modulating underlying phase-space structure, controllability, and observability of dynamical systems to enable more efficient learning and adaptive control.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an average of $1.25M per year for five years, supporting no more than six funded faculty researchers. Exceptions should be discussed with the topic chiefs during the white paper phase of the solicitation.

- For Topic 5, proposals are invited that include participation from Australian (AU) academic institutions; however, AU participation is not a requirement. In the case of proposals with AU participation, there still should be a single US primary institution and one PI submitting the overall proposal. Funding for the AU participation will be allocated separately by the AU government. Opportunities for Australian funding for such collaborative proposals are described at http://www.business.gov.au/ausmuri

Research Topic Chief: Dr. Samuel Stanton, 919-549-4225, samuel.c.stanton2.civ@mail.mil and Dr. Alfredo Garcia, 919-549-4282, alfredo.a.garcia31.civ@mail.mil

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Topic 6 (ARO): Coevolution of Neural, Cognitive, & Social Networks: Mind-Body-Community Connections

Background: Network science advances in social network analytics and brain connectomics allow for greater understanding of network effects impacting mood and brain states. New mathematical and statistical models allow for unprecedented analysis of information dissemination and decision making. Recent research shows the impact of complex interactions between people's behavior and the route of messages through their social networks with respect to smoking behaviors, obesity, and the spread of happiness. Likewise, studies exploring mindfulness show measurable impact on human behavior as well as communication patterns between several brain regions. With greater understanding of the impact of social network connections (such as family, friends, healthcare teams, and weak ties) on the behavior of individuals embedded in society, attention must be turned to developing a foundational science to quantify how individuals' bodies and minds are impacted by such social forces and vice versa. Collective advancements in tracking evolutionary network dynamics and applying complex systems theory approaches to understand structural and functional connectomic changes between brain regions may now be applied to further refine the definition of networks in the brain and the connection to outward social networks. Moreover, non-invasive neuroimaging is now being applied in social science studies with respect to individual and collective decision making. Advancements in these disciplines leave scientists poised for unifying research to study coevolutionary dynamics and state transitions in multilevel networks with varying temporal properties. Such research could provide a framework to elucidate the connections between the underlying individual brain functional connectomes and neuroplasticity, conscious and less-than conscious cognitive processes, biophysiological processes, and social influence mechanisms, and, ultimately, lead to a causal theory for mind-body-community connections.

Neuroscience advances in mapping human neural activity can now be combined with social and cognitive network research to understand how people are connected to others and the causal impact of messages from their social network on changes in their brain states. These advances are relevant to our understanding of individuals who suffer from a variety of conditions such as PTSD, depression, anxiety disorder, substance abuse/addiction, and fibromyalgia/chronic pain. Recent modalities showing great promise for helping people with such conditions include mindfulness and hypnotherapy. Simultaneously focusing on the coevolution of macro and micro level dynamics may identify underlying markers for causative mechanisms that hinder and/or promote healing as expressed through observable brain state transitions as a function of information received and processed. This coevolutionary dynamical approach will set the stage for the development of novel solutions to support a person's transition from illness to wellness.

Objective: The objective of this MURI is to identify and model the coevolutionary dynamics of neural, cognitive, and social networks as people transition between illness and wellness while engaged in rapid integration treatment modalities.

Research Concentration Areas: Suggested research areas include but are not limited to (1) an integrated, social science theory bridging neural, cognitive, and social networks; (2) a computational network approach and machine learning for pattern recognition and identification of dynamic functional connectomic interactions from non-invasive neurophysiology and neuroimaging data; (3) mindfulness and hypnotherapy modalities as applied to at least one of five conditions identified above; and (4) an integrated mathematical model for predicting and controlling state transitions of an

individual's neural, cognitive, biophysiological, and social networks.

Anticipated Resources: $1.25M/year for 5 years to support up to six funded faculty members.

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Topic 7 (ARO): Network Games

Background: Advances in scalable algorithmic techniques have made Game Theory a practical tool in a number of security related applications, especially in the context of adversaries and defenders modeled in a 2-party game. In practical situations, however, there are social networks that underlie adversarial and defender groups, respectively, with potential weak links between members of opposing groups which are effectively used by both groups to infiltrate the other. Examples include the use of double-agents in infiltrating gangs and non-state adversarial groups, targeting of weak members in herd of deer, targeting of specific T-cells in tumors, *etc*. The dynamics of networks on networks is an ill understood problem, especially the use of weak links in strategic decisions. Furthermore, there are situations, such as in modeling adversarial groups embedded in an ally's host population, where the need to consider multi-party interactions at multiple scales becomes important. The host population while agreeing that the adversarial group is a threat to society is nevertheless sympathetic to the issues

raised by the adversarial group. In such cases, an intuitive strategy might be to influence the sentiment of the masses while targeting individuals in the adversarial group with each success (or failure) of the defender resulting in a weakening (or emboldening, respectively) of the adversarial group.   A meaningful mathematical analysis would require a multi-scale framework in which both coarse grained model (eg. of the host population) and fine grained model (of the social network of adversaries) need to be reasoned about. Recent hand-curated work by Aaron Mannes (anthropologist) and V. S. Subrahmanian (computer scientist) on the adversarial group Lashkar-e-Taiba shows the efficacy of multi-scale modeling, and the need for a mathematical framework and compositional algorithmic techniques for solving massive games that arise in such security situations. Finally, limited success in solving Bayesian Network games, under the Network Science CTA by P. Basu and others, shows that the community is ready for larger challenges.

Objective: A new compositional Game Theory framework for characterizing dynamics of interaction between multi-genre networks that could potentially share members or have weak links. Furthermore, new multi-scale game theory modeling techniques are needed which allows (a) continuum and discrete models to co-exist, (b) modeling of cooperative and non-cooperative behavior, and (c) learning from game states and history, with attendant notions of approximation, refinement and equilibria that would drive formulation of algorithmic techniques for understanding dynamic, non-equilibrium states and characterization of equilibrium states.

Research Concentration Areas: Advances are necessary from a multi-disciplinary group which might include: (1) Probability and Statistics -- creation of novel probabilistic methods to analyze and potentially solve the stochastic process such as martingale methods and optimal transport, and a potential modeling with noncommutative probability theory; (2) Algebra/ Topology – characterization of approximations and semantic-soundness notions that allow transfer of results across modes and scales of multi-scale, multi-mode formulation of network games; (3) Machine Learning -- development of techniques that allow incorporation of real-time learning in game theory; (4) Computer Science -- algorithmic techniques for tractable data-driven analysis of non-equilibrium dynamics; (5) Social science -- social network analysis to understand and reason about non-state adversarial groups embedded in host nations that might sometimes be defender's ally. Policy formulation in dealing with non-state actors is an important problem for the military.

Anticipated resources: It is expected that $1.25M/year for five years would be available to fund not more than six university faculty researchers.

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Topic 8 (ARO): Modeling Interdependence among Natural Systems and Human Population Dynamics

Background: Large-scale environmental changes such as floods, earthquakes, and droughts, can drive social mobility, which often precipitates new population migration patterns that in turn affect health, crime, and sociopolitical instability as humans relocate to access critical resources. However, the ability to model, theorize, and predict the interdependencies among environmental change and human social system dynamics remains a scientific challenge.

Successful models of social-natural interdependence must account for the unique temporal/spatial scales of those systems, the factors determining action, and the natural and social constraints placed on those actions. These requirements pose substantial analytic challenges that no single discipline has been able to overcome. For example, prior research in the social sciences addresses how land, sea, and space perturbations affect poverty and civil unrest, but the tipping points in environmental change leading to

population migration and subsequent impacts are not understood. Although research in the environmental and geological sciences has addressed the role of policy on human-environment impacts, it is not an effective predictive model. Network science offers models of how social ties influence individual action, but networks are broken during environmental changes; thus, network analytics alone cannot yet address the problem of predicting mass migration. Social scientists can distinguish crowds (i.e., mass collectives of loosely connected people) from groups (i.e., collectives whose members know most others), but tend to view crowds as chaotic, which is an intractable modeling problem. Mathematicians and physicists have modeled the behavior of a variety of non-human groups as analogous to self-propelled particles, which include attraction and repulsion forces; yet, these models do not account for multi-level relationships in social behavior, such as the impact of social institutions.

Recent discoveries across multiple disciplines may provide the opportunity to create integrated, predictive models of natural-social system interdependence. Social scientists can now successfully model crowd behavior in particular conditions, such as the non-linear interactions of human oscillations around bottlenecks in pedestrian crowds. New discoveries in non-human species have documented critical factors in response to barriers and threats. Environmental scientists can now model intricate relationships tying land, sea, and atmosphere across different geographical and time scales. In addition, new historical and institutional data sets are available that document environmental changes and migration data (e.g., Hiroshima historical data, Wittgenstein Center data sets, United Nations research on refugee migration) that can serve as testbeds to aid in model development and validation.

Objective: The objective of this MURI is to create a theory integrating environmental change, human social system dynamics, and the corresponding interdependencies, to create and validate *predictive* models that capture these dynamics to anticipate the trajectory of environmental change and human effects on these changes.

Research Concentration Areas: Suggested research areas include, but are not limited to: developing and validating predictive models of **(1)** how environmental change affects the availability of critical resources; **(2)** how these extreme environmental and resource shifts impact populations (e.g., migration and settlement patterns) through natural and imposed barriers; and **(3)** how population dynamics affect both natural systems (e.g., resource changes) and social dynamics (e.g., crime, health crises, civil unrest). The work to understand these interdependencies spans (a) anthropology, sociology, political science, geography; and (b) mathematics, physics, environmental and geological sciences.

Anticipated Resources: $1.25M/year for 5 years to support up to six funded faculty members.

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Topic 9 (AFOSR): Physically Viable Learning for Control of Autonomous Dynamical Systems

Background: Future relevant DoD autonomous systems (e.g., cyber-physical, biological, neurological) will operate in contested environments and must be resilient to abrupt system changes. New control procedures and operational envelopes will be required that leverage the combination of learning techniques and physical laws with dynamical systems and control theory to provide real-time effective performance. In this context, learning is specifically the viable learning of the (change of) equations of evolution; as opposed to current techniques of learning and artificial intelligence techniques that require large amounts of training data. Recent research has showed that a number of physical laws, governed by PDEs/ODEs, can be discovered from datasets. Although these results have gone well beyond the identification of system properties that is typically tackled by data analysis techniques, some challenges remain: (1) for a small amount of data, the reconstruction of dynamical systems is non-linear and ill-posed; (2) due to the hybrid nature of the dynamics of many relevant systems, partial differential

inequalities or differential relations are involved, as opposed to merely PDEs or ODEs or their stochastic analogs; (3) in order to achieve recovery, a new dynamical model with bounded uncertainty along with its relevant subspace that is controllable (accessible) and observable (constructible) must be discovered quickly in finite time rather than asymptotically; (4) the weaker notion of viability versus invariants for hybrid systems inhibits straightforward calculation of solutions. Within this learning strategy, time to solution is itself part of the objective and it is bounded by the estimated times to critical failure (or impact), which must be re-evaluated as the search proceeds. Prior knowledge of physical laws and a-priori, "intelligent" information of the system's physical characteristics can accelerate the search. Finally, learning equations of evolution steered toward satisfying control objectives and the system away from bad behaviors (e.g., instability) is a key component of autonomy that has never been considered in depth.

Objective: To address the aforementioned challenges, this MURI topic calls for new theory from mathematics, engineering, and computer science to provide a mathematically rigorous methodology for quick learning to discover altered and new dynamical systems and their evolution. Theory should be scalable, observe physical laws, incorporate domain knowledge, and provide guarantees in the presence of structured and unstructured uncertainty. An additional research direction would be in new formulations for reachability and stability based on the newly discovered dynamical systems. The final product of the MURI is a theoretical foundation to discovering a physically traceable family of relations and maps so that evolution of the system can be predicted for the purposes of completing control objectives.

Research Concentration Areas: A new mathematical framework is requested on combining learning and data driven techniques with dynamical systems and control theory to provide new ways of learning changing dynamics and controls related subspaces such as observability, controllability and reachability and viability sets for autonomous dynamical systems in cases of large and abrupt changes. New perspectives from differential geometry, analysis, algebraic geometry and optimization are to be leveraged for development of computationally efficient algorithms that would not require use of large quantity of data which would not be available for the situations that are of interest.

Anticipated Resources: It is expected that awards under this topic will be an average of $1.5M per year for five years, supporting no more than six (6) funded faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

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Topic 10 (AFOSR): Nanoscale Vacuum Field Effect Transistors

Background: Despite the focus on solid-state electronics for computational applications, the transport of electrons in vacuum allows for velocities that are orders of magnitude higher than possible in the solid state; devices having femtosecond transit times can be realized when dimensions are on the nanometer scale, a scale that is now achievable through use of two dimensional (2D) and newer three-dimensional lithographic methods. Vacuum transistors and more-elaborate vacuum device concepts have been envisioned, employing integrated, voltage modulated electron sources based on vacuum field emission. Benefitting from advances in modern lithographic techniques, nanoscale processing technologies, and new electronic materials such as nanotubes, nanowires, graphene and other 2D materials, as well as advances in computational electromagnetics, transistors based on this concept have recently been demonstrated with remarkable results. The resulting vacuum devices could improve speed, power, radiation-resistance and thermal stability relative to solid-state devices. At atmospheric

pressure or possibly under modest vacuum, easily obtained with existing encapsulation methods, a sufficiently low collision probability between the electrons and gas molecules can be achieved because the anode-cathode gap is shorter than the mean free path of electrons in air.

In addition, these devices have been demonstrated to operate at low voltages, well below the first-ionization potential of most gases, presumably limiting the impact if such collisions take place. There are, however, many open questions and scientific challenges to address before the promise of these vacuum devices can be fulfilled. Standard field emission theory does not capture the detailed material properties that affect the electron density and does not properly calculate transmission probability for the smallest structures, and emission measurements typically show a variety of effects not predicted by theory. Better models applicable to structures at these physical scales and which include more detailed material properties, such as impurities, dislocations, band structure, and surface effects need to be developed. Successful devices should consider degradation mechanisms and reproducible and reliable manufacturability. Materials development, including self-assembly techniques and nanocomposites for tailoring of electric fields, may be required. While initial demonstrations of single devices are appropriate, one must also consider related circuit elements and the possible use of functional blocks. Fundamental differences between vacuum devices and solid-state devices, including, for example, the lack of complementary structures and the implications for standby power, may require a complete rethinking of how efficient and efficacious circuits should be designed.

Objective: The objective of this MURI topic is to advance the fundamental understanding of vacuum field emission in nanoscale field effect transistors (FETs) or similar devices, including rational materials and structural designs, toward the demonstration of discreet functional devices and circuits for future robust high-speed electronics.

Research Concentration Areas: Suggested research areas include: (1) vacuum field emission and surface physics; (2) vacuum electronics and integrated circuit design; (3) applied mathematics addressing effects associated with reduced scales in Maxwell's equations; (4) nano-manufacturing of suitable materials and devices consistent with tunneling and field emission; and (5) characterization of nanostructures, transport properties, and degradation mechanisms.

Anticipated Resources: It is anticipated this topic requires approximately $1.5M per year for 5 years, supporting approximately six (6) funded faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

Research Topic Chiefs: Dr. Jason A. Marshall, Plasma & Electro-Energetic Physics, AFOSR/RTB-1, 703-696-7721, jason.marshall.3@us.af.mil, Dr. Kenneth C. Goretta, Electronic Materials & Devices, AFOSR/RTA-1, 703-696-7349, kenneth.goretta@us.af.mil

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Topic 11 (AFOSR): Molecular-scale Studies of Liquid-Solid Interfaces in Electrochemical Processes

Background: Electrochemical processes are critical to many energy storage modalities including batteries, fuel cells, and chemical storage of electrical energy in chemical bonds, as in the conversion of CO_2 and sunlight into liquid fuels. The processes that control the important physical, chemical, and materials behavior in many of these systems occur at liquid-solid interfaces, which can be quite complex due to, for example, the evolving nature of the interface, large interfacial electric fields, ion diffusion and mobility, and solvent reorganization and dynamics. Information about the intermediates and critical steps in the chemical transformations that determine the selectivity and energy efficiency in electrochemical systems is now often inferred from observation of bulk behaviors such as in cyclic voltammetry, spectrochemical product analysis and electrode microscopy. Molecular-scale probes that can provide detailed microscopic and spectroscopic information with the molecular specificity needed

to unambiguously detect and characterize intermediate species and processes would greatly advance this field if they can operate in the complex interfacial environment present in real electrochemical and electrocatalytic systems. Recent advances in optical and surface-sensitive spectroscopic techniques, such as the use of sum-frequency generation and related methods to probe important interfacial systems, combined with emerging ab initio and statistical molecular-level simulation methods capable of describing chemical transformations at complex interfaces can create a qualitatively new and important way to address this regime. These new molecular-level diagnostic and simulation tools can help provide a better understanding of reaction mechanisms and factors controlling over potential and selectivity in electrochemical processes, model electron and proton transfer at surfaces, and elucidate the effects of interfacial fields and solvent dynamics at electrochemical double layers. It is therefore timely to launch a concerted effort to integrate experimental and theoretical approaches to provide the fundamental scientific information needed for the improved rational design of electrochemical processes that will greatly enhance energy storage methods.

Objective: We seek the development and concerted application of new molecular-level spectroscopic and simulation methods to detect and characterize the identity and structure of intermediate species and to elucidate the important reactive and energy transfer processes in electrochemical systems of importance to energy storage and utilization.

Research Concentration Areas: Areas of interest include, but are not limited to: (1) Development and application of spectroscopic methods for the *in situ* or operando identification of intermediates in electrochemical and electrocatalytic processes in real time; (2) Development and application of molecular simulation methods to identify the dynamic behavior of solvent motion and reorganization at and around electrodes and identifying their effects on electrochemical and electrocatalytic processes; (3) Studies of the real-time kinetic and dynamic behavior occurring at solid-liquid interfaces and electrochemical double layers in electrochemical processes; (4) Studies of electron and proton transfer and the role of interfacial fields at electrodes in electrochemical and electrocatalytic processes.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an average of $1.5M per year for 5 years, supporting no more than eight (8) funded faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

Research Topic Chief: Dr. Michael R. Berman, AFOSR, 703-696-7781, michael.berman@us.af.mil

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Topic 12 (AFOSR): Electromagnetic Non-reciprocity via Temporal Modulation

Background: Research in metamaterials and integrated photonics has been rapidly evolving, offering today versatile platforms to realize various artificial structures with properties that go well beyond what was obtainable with natural optical and microwave materials for a variety of technologies. For example, some novel properties of photonic nano- and micro-structures are based on arrays (periodic or random) of resonant inclusions that locally enhance light-matter interactions. Some other unique features are related to strong and controllable spatial or temporal dispersion. So far their practical impact on optical and microwave technology has been hindered by losses, bandwidth limitations, and often prohibitively large dimensions (especially thickness). Yet another fundamental limitation has been related to the lack of timely reconfigurability of photonic and microwave structures. A number of recent theoretical and experimental studies suggest that the use of time-dependent modulation has the potential to overcome these limitations and thereby revolutionize integrated photonics and opto-electronics. Of particular interest is the possibility to mimic nonreciprocal magneto-optical effects using temporal modulation of physical parameters of photonic and microwave structures. Such a dynamically induced electromagnetic non-reciprocity can eliminate the need for lossy magneto-optical materials and bulky DC magnets and can lead to a new generation of compact and energy efficient isolators, circulators,

phase shifters, and other non-reciprocal optical and microwave devices. The time dependent modulation can be laser-induced or it can be provided by some other electromagnetic oscillations or by electric current. It can be also realized via acousto-optical or opto-mechanical interactions. In addition to non-reciprocity, temporal modulation can provide localized gain for light amplification and lasing, as well as for up- and down- frequency conversion. The ultimate goal is to overcome the fundamental limitations of the currently fielded non-reciprocal and possibly nonlinear optical and microwave devices and, at the same time, to unlock qualitatively new phenomena in the areas of active, non-reciprocal and nonlinear photonic structures.

Objective: Exploration of a new class of photonic structures in which strong electromagnetic non-reciprocity, reconfigurability, and other desirable features are achieved by means of controllable temporal modulation, periodic or otherwise. Broadband and/or multi-spectrum performance is desirable. The goal is to overcome fundamental physical limitations of current approaches in integrated photonics and find better alternatives to existing microwave materials, photonic structures, and magneto-optical devices. This research will also unlock new phenomena in the area of wave propagation and scattering in media subjected to time-dependent modulation. A multidisciplinary research effort will bring together physicists, electrical engineers, material scientists, and mathematicians to explore new physical ideas and engineering concepts, as well as to design, fabricate, and test novel devices.

Research Concentration Areas: Areas of interest include, but are not limited to: (1) exploring new physical phenomena in microwave and photonic structures subject to time-dependent modulation; (2) developing novel applications of such structures including conceptual design of compact and energy efficient non-reciprocal devices, conceptual design of photonic structures for parametric light amplification and lasing, conceptual design of integrated photonics for dynamically controlled response with active feedback, and conceptual design of integrated microwave/photonic devices for beam formation and steering; (3) experimental implementation of such material platforms for optical and microwave applications.

Anticipated Resources: It is anticipated that awards under this topic will be no more than $1.5M/yr for 5 years, supporting no more than six (6) funded faculty members. Exceptions warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

Research Topic Chief:
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Topic 13 (AFOSR): Heterogeneous Interfaces: Route to New Optoelectronic Properties

Background: The properties of a hybrid thin film heterostructure are often dominated by the interface between the constituent materials that comprise the structure. Extensive research has revealed key mechanisms and material properties that control an interface between chemically similar, isostructural materials (e.g., oxide-oxide, semiconductor-semiconductor). Integrating thin films with dramatically dissimilar chemical bonding, crystal symmetries and electronic structures, represents a promising new approach to engineer novel functional materials. This topic is motivated by recent success in integrating chalcogenides with oxides, such as superconducting FeSe on $SrTiO_3$, and combining complex oxides with semiconductors, such as $BaTiO_3$ on Ge, thus synergistically combining functional properties. For instance, in ferroelectric heterostructures, capitalizing on the reversible polarization of the ferroelectric, facilitates the implementation of optical nonlinearities and carrier modulation at extremely high carrier densities. Advanced vapor deposition techniques, such as molecular beam epitaxy, allow the requisite control over the interface composition necessary to integrate epitaxially, chemically, and structurally dissimilar materials. Recent advances in synchrotron-based diffraction and X-ray absorption

spectroscopy enable elucidation with picometer precision of both physical and electronic structures at dissimilar interfaces. Coupling advanced growth and characterization techniques with the predictive power of first-principles calculations, offers a powerful approach to design and create materials with superior and perhaps multifunctional performance for nonlinear electronic switches, high- temperature superconducting circuits and optical devices.

Objective: The objectives of this experimental and theoretical MURI topic are (1) to discover and engineer novel functional properties arising at heterogeneous interfaces and (2) to establish design rules from first-principles calculations and state-of-the-art growth techniques. The result will be materials with broad application to nanoscale circuits that capitalize on large nonlinear susceptibilities unique to hybrid interfaces. Microwave and electronic applications using interfacial superconductors and photonic applications with integrated electro-optic modulators are among the topics of interest. This subject focuses on dissimilar classes of materials (e.g., selenide-oxide, oxide-Si, Ge, or compound semiconductor), as distinct from hybrid materials comprised of similar materials (e.g., oxide-oxide, Si-Ge, GaN-AlN). To provide sufficient depth, proposers have the option to consider only one type of heterogeneous interface.

Research Concentration Areas: The research concentration areas include materials systems in which the properties are dominated by heterogeneous interfaces. Examples of dissimilar material interfaces include the following: (1) epitaxial growth of $Mg_xCa_{1-x}O$ on GaN by Atomic Layer Deposition; (2) oxide-semiconductor interfaces (e.g., $SrTiO_3$-Si, $SrTiO_3$-GaAs, $BaTiO_3$-Si, $BaTiO_3$-Ge) that are technologically relevant for electronics and photonics. This approach directly couples the polarization of a ferroelectric, such as $BaTiO_3$, to the properties of a semiconductor. In addition, with its enormous optical nonlinearities, $BaTiO_3$ and related compounds can serve as a key component for hybrid semiconductor-photonic systems.

Anticipated Resources: It is expected that awards under this topic will be an average of \$1.5M per year for five years, supporting no more than six (6) funded faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

Research Topic Chiefs: Dr. H. Weinstock, AFOSR/RTB, 703-696-8572, harold.weinstock@us.af.mil; Dr. K. Goretta, AFOSR/RTA, 703-696-7349, kenneth.goretta@us.af.mil

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Topic 14 (AFOSR): Piezoelectric Nanoenergetic Materials with Adaptable and Tailorable Reactivity

Background: Energetic materials can respond to internal and external fields (thermal, electrical, magnetic, stress, etc.) but their coupling characteristics are neither adequately understood nor designed for utilization. This MURI topic aims to utilize coupling characteristic of polyphase energetics using piezoelectric effect and aims to address two major challenges, tailorable reactivity and adaptability. In recent work[1], energetic composites of nanoaluminum and a piezoelectric polymer were shown to have interesting properties, including the ability to ignite following shear manipulation, store electrical charge, and be sensitized to ignite at lower impact energies by applying a voltage. Piezoelectrically reactive phases could also be designed to act as embedded sensors that could be monitored for exposure to vibration or acceleration history, thus providing important information on the health monitoring. In this context, the piezoelectric phase can be a continuous active phase within a higher-volume phase of nanonergetics or matrix; it can be described as an *in-situ* composite. Piezoelectric reactive materials could potentially be fabricated to create sensitizing voids on external command, transforming an insensitive propellant into an impact-sensitive material or be designed to activate at reactive surfaces to enhance or inhibit reaction, and thus burning rate. Fundamental studies are needed in order to achieve externally controlled and adaptable energetic materials that could result in disruptive ranges (orders of

magnitude) in reaction rates. In the hearth of the proposed topic is the science based design of composite structures through manipulating molecular compression that reduces the energy gap between the highest occupied and the lowest unoccupied molecular orbital, resulting in local metallization and ignition[2]. In this context, the role of active piezoelectric phase and interfaces is pivotal for the understanding and control of hot spot formation of energetic materials, thereby affecting ignition and propagation mechanisms[3]. The challenges associated with the multifunctional composite structure require design of polyphase materials in mesoscale comprising the structurally robust nano-energetic phase and functional piezoelectric phase. These materials can be fabricated to be highly electroactive.

Objective: This MURI addresses the fundamental processes of local energy transformations within condensed phase piezoelectric reactive nanoscale materials and their control to directly impact material characteristics such as reaction rates, energy storage, and sensitivity. The ability to interrupt and alter these properties on molecular timescales is of interest as is the understanding and characterization of the mechanisms by which such control or tailored design is achieved.

Research Concentration Areas: The fundamental challenge is two-fold: First challenge, design piezoelectrically activated nano-energetic composite materials that possess attributes beyond the basic energy release or ignition properties. Emphasis should be on understanding of energy transformation, energy flow, energy repartition, phase change, electromagnetic effects, and charge dipole energies in polyphase materials. Second, develop the scientific underpinning of electromechanical properties from first principles, and couple these atomistic properties through mesoscale physics and chemistry of piezoelectric domain walls. In order to advance the theoretical description of the interface and design experimental approaches to quantify coupling of fields, predict properties, and control responses to various stimuli, a synergistic experimental-theoretical approach will be required.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an average of $1.5M per year for 5 years, supporting no more than six (6) funded faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

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Topic 15 (AFOSR): Advanced Mean-Field Game Theory for Complex Physical & Socio-Economical Systems

Background: New mathematical concepts are being developed for understanding the behavior of large, complex systems, found in both natural (e.g. global climate, genome, human brain or ecological networks) and artificial environments (e.g. computer networks, air and ground transportation, power grid), as well as in less tangible but still very important cases, e.g. socio-economic networks. Self-organization, emergent behavior and cascading effects can be typical characteristics of such systems, which are increasingly relevant to the DOD. Their modeling can be especially challenging, due to the

combination of multiple scales (temporal, spatial, or other variables) with different dynamical behavior (i.e. "multi-physics") and a network topology which is itself a dynamical variable. Real life complex systems can also resist the traditional approach of decomposition into smaller, weakly-correlated sub-systems that can be solved in parallel. A promising approach to complexity modeling relies on the sampling of a high number of interacting agents, with specific rules of behavior. Despite their relative simplicity, these models have been successful in various applications, e.g. economics, traffic flow management, or urban planning. More sophisticated and realistic individual agent behavior could be accounted for by translating psychological concepts or socio-economic data (for human-human or human-machine interactions) into mathematically rigorous principles. For a small enough network, the multi-agent dynamics are solvable via direct simulation. In the opposite ("thermodynamic") limit, mean field game (MFG) theory has become a powerful and promising powerful approach in which, similarly to the mean-field approximation in statistical physics, the leading order interaction is between an individual agent and the statistical average of all other agents. However, a real system has a large but finite number of agents, and one must account for finite size effects with associated (large) fluctuations. In addition to an assumed basic, rational behavior with appropriate cost functions, the interaction rules also include some stochasticity, from imponderable (irrational) agent-based or clique-based psycho-sociological tendencies, or from parametric uncertainty in complex engineering systems.

Objective: This MURI will develop a comprehensive and scalable mathematical approach to multi-agent dynamics, non-linearly coupled to the geometry of their network, and with the ability to incorporate detailed and rigorous rules of behavior, drawn from the abstraction of human psychology and group social behavior, or physical dynamics, constraints and control principles. The ideal global simulation capability would therefore target human and human/machine networks, but be equally be applicable to the engineering and design characteristics of platforms, transport networks, cyber-networks, or natural systems of interest to the DOD. The mathematical principles must also lead to scalable algorithms for rapid computations.

Research Concentration Areas: The approach must go beyond the zero[th] order of MFG. The stochastic differential equations (SDE) for agent trajectories, or their continuous counterparts, need to be generalized to include memory effects as well as psycho-/socio-mathematical models of rational and irrational agents. Geometry and topology must be treated as dynamical variables, non-linearly coupled to agent density or higher-order moments. Multi-scale (e.g. local rules) and non-equilibrium effects (e.g. cooperative equilibria) must be examined. Areas of potential research include, but are not limited to; dimensionality reduction of the strategy space, optimal transport theory, fractional-order transport equations, perturbative and Mori-Zwanzig expansion, or leveraging other concepts from many-body physics, e.g. renormalization group. **Anticipated Resources:** It is expected that awards under this topic will be an average of $1.5M per year for five years, supporting no more than six (6) funded faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

AFOSR Research Topic Chiefs: Dr. J.-L. Cambier, jean_luc.cambier@us.af.mil, 703-696-1141; Dr. B. Knott, benjamin.knott.2@us.af.mil, 703-696-1142; Dr. F. Leve, frederick.leve@us.af.mil, 703-696-9730; Dr. T. Nguyen, tristan.nguyen@us.af.mil, 703-696-7796

Topic 16 (AFOSR): β-Ga$_2$O$_3$ as a High-Critical Field Strength Material for Power Systems
Background: Oxide materials may reshape the frontiers of electronics and enable new capabilities for monolithic power, RF and electro-optic integration. β-Ga$_2$O$_3$ was developed as a lattice-matched, transparent, conductive substrate for GaN optical applications and has a wide-bandgap (4.9 eV) that is exceeded only by diamond and AlN. The large critical field strength (8 MV/cm) and wide range of n-type doping (10^{13} cm^{-3} – 10^{20} cm^{-3}) offers high performance power switching and RF capability that are pivotal for a wide range of DOD missions. The recent discovery of bulk β-Ga$_2$O$_3$ growth by

conventional techniques to achieve scalable substrate materials offers a growth platform for power switching devices with unprecedented performance. Several critical breakthroughs have been achieved for β-Ga$_2$O$_3$ technology toward RF and power switch applications such as 1 kV vertical Schottky diodes, critical field strength > 3.8 MV/cm, high current density > 500 mA/mm, lateral breakdown voltages > 700 V and enhancement mode wrap-gate transistors. These are remarkable metrics from first generation material system with immature structural knowledge, transport, and interface knowledge.

A comprehensive study of β-Ga$_2$O$_3$ structure is required to explain the role of the distortion of tetrahedral and octahedral sublattice sites in the context of these superior properties as compared with the meta-stable hexagonal α-phase. Atomistic simulation, materials synthesis, dielectric formation, interface studies, defect characterization, and thermal physics under high fields are required in order to fully realize the capabilities offered by the β-Ga$_2$O$_3$ material system. In addition, pushing this class of materials into extreme environments (in terms of temperature, electric field, and frequency) requires a more fundamental understanding of charge transport phenomena, especially at heterogeneous interfaces. In turn, this may guide and uncover new multicomponent β-Ga$_2$O$_3$ materials which can facilitate kilo-Volt class lateral power switch operation and mega-Volt class vertical switches that are not possible with any other material system.

Because β-Ga$_2$O$_3$ can be grown from a melt, it has the potential to be disruptive with revolutionary power switching properties at a fraction of the cost of existing technologies. Additionally, optoelectronic applications exist for deep-ultraviolet (DUV) wavelengths that enable DOD relevant sensing technologies such as biological and chemical agent detection and observation of DNA and proteins.

Objectives: We will develop the fundamental physics to understand carrier-defect interactions at extremely high electric fields and high temperatures, and explore the physical properties of bulk β-Ga$_2$O$_3$ and related alloys. We seek to understand the role of the monoclinic sublattice distortion in β-Ga$_2$O$_3$ and related shallow- and deep-level intrinsic and extrinsic defect impact on robustness. We will also explore directional dependencies of carrier transport and use that understanding to design and fabricate heterostructures and dielectric stacks to optimize transport properties for unipolar and/or bipolar operation.

Research Concentration Areas: Research concentration areas include, but are not limited to (1) theoretical studies of β-Ga$_2$O$_3$ and other polymorphs of Ga$_2$O$_3$, validation of structure using spectroscopy and microscopy; (2) first-principles modeling of defects, interfaces, and effects of various applied fields and their relations to time dependent properties; (3) modeling of layered architectures, including coupled conduction of the various carriers; and (4) design and characterization of heterostructures and prototype devices with nanoscale control of composition and structure. The combined communities of solid-state physics, chemistry and materials, and theory and multiscale modeling are needed for the scope of this effort.

Anticipated Resources: It is expected that awards under this topic will be an average of $1.5M per year for five years, supporting no more than six (6) funded faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

Research Topic Chiefs: Dr. Ali Sayir, AFOSR, 703-696-7236, ali.sayir.2@us.af.mil

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Topic 17 (ONR): Predicting and Validating Pathways for Chemical Synthesis
Background: Recent advances in computational chemistry now allow one to identify new, thermodynamically stable compounds having preselected and highly desirable properties. However, there is a problem in that the multistep processes needed to make those compounds can be very

complicated or unpredictable, and, those procedures are typically done on a trial-and-error basis. Promising compounds may never be synthesized even in small quantities for property evaluation, let alone establishing methods for a viable industrial scale production. Improvements in predictive synthetic strategies are required.

Synthesis planning software has been desired for many years[1] and attempts to create robust algorithms to assist chemists have been published and even marketed starting from the late 1960s.[2] None of those have been widely accepted by the synthetic chemistry community. There are two major problems with the current approach. First, they rely on databases of known chemical reactions and those databases are profoundly flawed, not because of the data they contain, but because of what they do not contain. More specifically those databases and the literature upon which they are founded include only successful chemical reactions; excluded are unsuccessful reactions.[3] This is due in part because journal editors and peer reviewers have not permitted publication of unsuccessful reactions and in part because the researchers themselves have viewed non-compliant chemical reactions as failures that don't merit dissemination. Accordingly, the data used for developing heuristics for synthesis planning is biased and can be misleading. Second, because many of the existing algorithms are based on a corpus of existing knowledge, they are incapable of predicting completely new reaction mechanisms.

Objective: This MURI program focuses on ways of overcoming those problems. We seek new theories, algorithms and protocols based on quantum chemical computing that can be used de novo or concurrently with existing synthesis planning methods to map out chemical pathways. This quantum-based approach is required to predict: (i) thermodynamics of initial reagents and final products along with all possible intermediates along the various reaction coordinates, (ii) kinetic rates of each step along those pathways, (iii) the influence of solvents, catalysts, salts and other common additives such that correct stereo and regioselectivites are predicted, (iv) reaction yields. Other non-quantum based approaches to reach our objective will also be considered.

Research Concentration: The focus of this effort should be on photochemical reaction planning. The reasons for this are: (a) high energy photon-driven reactions allow for the creation of highly strained ring systems that are otherwise hard to create; (b) there is relatively little known about excited state synthetic processes compared to ground state chemistries. The selected MURI team is expected to: (i) provide a general strategy for synthesis planning that accounts for all intermediates along the myriad pathways leading to a given target molecule, (ii) select a set of target molecules that may be of value to DoD and (iii) prepare and identify those products to establish that the synthesis planning strategy works. We expect a balanced effort that includes: (1) synthetic chemistry/materials science; (2) computational chemistry/materials science; (3) applied mathematics or computer science; (4) chemical analysis.

Anticipated Resources: Awards under this topic will not exceed an average of $1.5M/year for 5 years, supporting 4 to 6 faculty researchers. Exceptions warranted by specific proposed approaches should be discussed with the topic chief during the white paper phase of the solicitation.

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Topic 18 (ONR): Synthetic Microbial Electronics
Background: Synthetic biology (SynBio) has enabled new approaches and tools for sensing, energy

production and synthesis of high value materials. The field has also yielded genetically encoded methods for computation, signal processing and biological equivalents of many electrical circuits (e.g., amplifiers, oscillators, counters). Given the inspiration that electrical engineering has had on SynBio as a field, it is not surprising that focus on biologically-synthesized electronic materials and components has been growing[1]. Biological self-assembly enables complex nanometer-scale structures with impressive rates and energy utilization, e.g., $\sim10^{18}$ molecules/sec (equivalent to 5 sec for a 1GB chip), and energy utilization about 100x less than that of conventional subtractive manufacturing. If living microbes could be programmed to build and power actual electronic components, circuits and devices, novel paradigms for distributed sensing networks, energy management in ultra-low-power systems, and aqueous-based, ambient-temperature electronics manufacturing may be realized. This goal will require microbes to produce and organize electronic materials at the nano/micro-scale; build, test and/or repair electronic components and circuitry, and have the ability to generate electrical current to power the fabricated electrical devices

In nature, several microbial species interact directly with metals and minerals and have evolved mechanisms for forming intra-/extracellular crystals, fibers, composites and even hierarchical 3D structures[2]. "Electricigenic" microbes have evolved mechanisms to utilize, store, and generate electrical current[3,4]. Thus, these microbes can interact directly with mineral substrates, electrodes, and other cells, over multiple length scales (nm->cm). Electricigens (eg., *Geobacter*, *Shewanella, etc*) are genetically tractable, and may be useful bioelectronic "chassis" organisms for these SynBio studies; alternatively, well understood 'parts' from these organisms can be used to make non-native electricigens[5]. Indeed, native and non-native electricigens have been shown to function as microbial transistors, to express proteins that act as capacitors or voltage sensors[6], and produce current in response to external cues[7]. A variety of natural and engineered, self-assembling biomolecular scaffolds that can organize metals and other moieties into complex 3D architectures with nanoscale resolution have been described[8], but microbial production of these scaffolds has been understudied. Lastly, microbes have been metabolically engineered to synthesize various organic polymers including polyamides, polylactones and polyesters, and have the potential to synthesize conducting polymers (including conductive protein pili[8]).

This topic aims to support basic research to enable microbes to synthesize, test, and repair electronic materials, and to participate as active and programmable components in electronic circuit or device fabrication and powering.

Objectives: To explore SynBio-enabled synthesis, sensing, and control of microbial or microbially-produced electronic materials, circuits, and components; and to create a framework for describing and modeling properties of assemblies of these bio-electronic 'parts.'

Research Concentration Areas: (1) Microbial synthesis of organic, inorganic or hybrid electronic materials and components (e.g., conducting polymers, semiconductors, low-k dielectrics, nanowires, diodes, transistors); (2) Fabrication techniques and design tools that utilize living microbes to self-organize electronic materials into functional components and circuits; (3) Programming microbes to detect, test and repair defects in electronic materials/devices, and to power these devices; (4) Nanoscale characterization tools to elucidate the properties and behavior of bio-electronic materials and living microbial components.

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Topic 19 (ONR): Automated Technical Document Comprehension

Background: Current techniques for knowledge retrieval from a document primarily rely on statistical extraction and correlation of keywords or a set of grouped keywords. While these techniques can provide information on identifying the subject of a document, they fall short in providing an understanding of a document's content. Technical documents, such as scientific journal articles or engineering design documents, often contain entities such as diagrams, formulas, pictures, graphs, charts, and tables with associated captions, in addition to text descriptions. These additional entities can be essential for determining the content of the technical document. Humans typically gain understanding of the content of a technical document from understanding these entities and their relationship to each other and the associated text, coupled with their basic knowledge of the technical subject area.

Automated technical document comprehension will require recognition, understanding, semantic association, and information synthesis of text, related technical entities, and background knowledge. This will require methods and tools capable of extracting the semantic content, structure, and knowledge from a given document, thus enabling faithful and accurate knowledge acquisition from both the text description and the technical entities (i.e., diagrams, charts, tables, etc.) contained within the document. Ultimately, digital curation of document knowledge into a queryable library will enable knowledge acquisition, correlation, and discovery to support semi-automatic and automatic literature-based exploration for facts and solutions.

Objectives: The objective of this MURI is to investigate and develop principled approaches and computational methods for automatically extracting the semantic content, structure, and knowledge from a technical document encompassing both text and related technical entities (diagrams, charts, tables, etc), and the association between the text and these entities. In addition, an ability to meaningfully combine related content into a new document would be considered a significant advancement of the state of the art.

Research Concentration Area: This MURI is focused on extracting and understanding the technical content of any technical document. Suggested research areas include, but are not limited to: (1) recognition of semantic objects from diagrams, charts, tables, etc. and textual descriptions, (2) semantic

contextual linkage among various objects and their attributes within various modalities (e.g., graphical, textual, tabular, etc.), (3) integration/fusion of information extracted from various modalities into coherent technical knowledge representation, (4) automated synthesis of a new technical concept or design based on a set of existing literature within the topic area. A resultant capability is the ability convey to a viewer who has not read the document what the document is about and show the contextual relationships.

This MURI topic is intended to go beyond strictly indexing and retrieving snippets of knowledge to be integrated with an existing knowledge base. Statistical correlation and big-data only approaches will not be considered competitive for this MURI.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an average of $1.5M per year for 5 years, supporting no more than eight faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chiefs during the white-paper phase of the solicitation.

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Topic 20 (ONR): Materials for Smart Multifunctional Superstructures [(MS)^2]

Background: Advances in materials synthesis have enabled remarkable design and control of material properties and functions at the nano- and mesoscale. However, this materials development has thus far focused almost exclusively on realizing material architectures with a single optimized function or property, which can then be integrated to combine the functionalities. Larger-scale inherently smart multifunctional superstructures, in which the material itself senses and responds to its environment, have remained largely unexplored. Ultimately, the desired design is a material where multiple specific functions are completely integrated with auxiliary utilities, such as sensing, actuation and power, and are mutually present throughout the material volume at the scale of a few microns. The envisioned smart multifunctional superstructures are expected to enable material characteristics not available today, such as self-adapting material hardness, self-adjusting thermal conductance, and self-controllable hydrophobicity and -philicity.

The vision of creating smart multifunctional material superstructures with self-adjusting properties by integrating nanoscale building blocks (e.g. 2D and 3D materials) leads to some intriguing scientific questions and challenges. First, the performance of the nanoscale elements needs to be integratable, i.e., the nanoscale property and function must be preserved in the superstructure. Smart assembly of the nanoscale components should provide collective enhancement of the superstructure properties through component-to-component interaction. The latter will be of critical importance in integrating the various utilities in the material and will require thorough understanding of the assembly process in order to control short- and long-range order in the superstructure. Second, the dissimilar chemical and thermodynamic stabilities of nanoscale building blocks with single functionalities present a significant challenge to designing a superstructure with fully integrated, self-adjusting mechanical/electrical/optical/thermal/etc properties. Understanding the limits imposed by specific material chemistries will be integral for designing appropriate assembly mechanisms.

The complexity of these new materials systems will require a close interaction between computational materials science and chemical synthesis. The enabling science to address these challenges will provide a powerful new capability for designing and integrating new nanoscale materials and smart superstructures.

Objective: To establish a scientific capability for the design of smart multifunctional material

superstructures with multiple utilities (>2) fully integrated and mutually present at the micron scale.

Research Concentration Areas: Areas of interest include but are not limited to: (1) Materials science and chemistry to enable assembly and integration of nanoscale building blocks to create smart multifunctional superstructures; (2) Approaches to fully integrate multiple functionalities in a mutually present fashion within a material volume and to understanding the range and limits for each functionality within the smart multifunctional material superstructure; (3) Integrated Computational Materials Engineering to support design of nanoscale materials building blocks and smart multifunctional material superstructure systems; (4) Design of smart multifunctional superstructure systems, optimized for specific functions in multiple (>2) areas that may include structural composite, optical , electronic, dielectric and thermal behavior.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an average of $1.5M per year for 5 years, supporting no more than six funded faculty researchers. Exception warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

Research Topic Chiefs: Dr. Antti J. Makinen, ONR Code 332, antti.makinen@navy.mil;
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Topic 21 (ONR): Advanced Optical Materials that Create Force from Light

Background: Optoelectronic interactions, where charge carriers move in conduction and valence bands as a result of photonic excitation, have been exploited for decades, serving as the foundation for many modern optoelectronic devices. However, research in optomechanical response, where light stimulus produces dimensional changes (strain) in materials, is emergent and offers future applications for high-bandwidth, high-resolution actuators or coupled adaptive sensor systems. Today, fiber optic wave guides transfer kilowatts of light energy over kilometers with very low transmission loss. But current approaches for converting light energy into mechanical work (e.g. a light driven photocell running a solenoid) suffer from multiple, compounded conversion losses, where direct photo-mechanical coupling could eliminate these inefficiencies. Materials for optically-coupled mechanical actuators are currently at the nano- and microelectromechanical systems (MEMS) device-scale, producing only limited potential strain energy (or force) in photonically-driven systems. Optoacoustic coupling has been demonstrated in materials illuminated with high intensity lasers pulses, and has power transduction through photo-piezoelectric effects has been shown to produce oscillator frequency changes, but offer limited applications. Targeting direct energy conversion based on optomechanical coupling at a molecular level could offer research gateways leading to new, fast photo-mechanical actuators. However, the exact mechanisms (and repeatability) of photo-induced chemical and other physical changes remain unclear and debatable in the known optomechanically active materials. Understanding these complex interactions of photons with materials is key to forming the underlying framework for material selections in creating reversible structural, chemical, or dynamic changes necessary to realize new lightweight actuation mechanisms and sensors powered by light energy

Objective: This MURI seeks to invigorate innovative research to understand the atomic, molecular, and bulk interactions of materials with light and create a fundamental framework describing optomechanical physics, thermodynamics, and material sciences associated with photonic conversion and transport phenomena that produce repeatable strain energy at nano/micro and macroscopic scales.

Research Concentration Areas: (1) Theoretical computational modelling of the reversible optomechanical interaction both   at the atomic and molecular level and at the meso- and macroscale ; (2) Design and discovery of new optomechanical materials and material architectures through chemical

synthesis and material engineering;   (3) Experimental investigation and characterization of photo-reactive materials, coupled or uncoupled with suspensory materials; (4) Integration of photon sources with photomechanical architecture.

Anticipated Resources: Anticipated award(s) made under this topic are expected to be no more than $1.5M per year for 5 years (on average), and supporting no more than six (6) funded faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chiefs during the white paper phase of the solicitation.

Research Topic Chiefs:
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Topic 22 (ONR): In situ Microstructural and Defect Evolution below the Micron Scale in as-Deposited Metal Alloys

Background: Fundamental material challenges limit the full realization of Metal Additive Manufacturing (AM) technology. We currently lack sufficient knowledge of the highly dynamic and inherently complex thermomechanical processes in AM, which induce stark differences in microstructural and defect evolution, in contrast to traditional manufacturing processes. AM has very rapid heating and cooling/solidification rates that are orders of magnitude faster than those observed in conventional processes. Repeat heating of prior passes during layered buildup also uniquely affects microstructural evolution. It has been shown that macro material properties for as-deposited alloys –that exhibit similar microstructure– may be significantly different, pointing to the need for more sensitive analysis at smaller length scales. Additionally, AM processes may cause severe residual stress, variation in mechanical and corrosion properties, selective evaporation of lower vapor pressure volatiles, and selective elemental segregation at surfaces and grain boundaries that significantly challenge our ability to discover accurate process-microstructure-property-performance models for AM. To greatly assist in elucidating how variations of microstructures at the micron down to angstrom length scales, enhanced in situ characterization techniques is needed to understand the metallurgical phenomena that effect resulting material properties. As an example, the use of high brilliance synchrotron X-rays provides penetrating capability for rapid in situ / high temperature experiments. Coupling experimental techniques with computational physics based models will be necessary to aid in guiding and interpreting the experimental data.

Objective: A fundamental understanding of AM is needed to enable future, locally tailored materials to achieve material performance at spatially critical points. In order to achieve this long range goal, we need to be able to understand the impact of, for instance, contaminants/dopants, dislocation behavior and localized crystal strain fields on microstructure and defect evolution in AM materials as a result of cyclic processing. In order to achieve this understanding, we need to answer the following scientific questions: (1) How do contaminants/dopants affect vacancy and interstitial behavior at microstructural interfaces of AM materials? Highly concentrated cyclic heating can cause local elemental vaporization during the process and subsequently vary alloy composition in the fabricated geometry. (2) How does dislocation behavior evolve through an AM process? The rapid thermal cycles and phase transformations will affect dislocation formation, annihilation and movement in the lattice structures and interfaces. (3) How do thermally activated defects drive phase transformation behavior in as deposited or post-processed AM materials? Answering these fundamental questions can enable correlations to the resulting micro and macro material properties. This provides critical fundamental information for the advancement of computational phase field AM models and understanding mesoscale behavior for an integrated computational materials engineering (ICME) approach.

Research Concentration Areas: Suggested research areas include, but are not limited to: (1) development of new theory and models to help elucidate fundamental mesoscale behavior and the influence of grain boundaries and thermally activated defects on various property-microstructure-performance relationships, (2) emerging in-situ/in-operandi characterization tools to differentially probe local lattice structures, smaller grains, larger grain sizes, and microstructural responses to various thermal and mechanical stimulae, and (3) design/validation of computationally-guided experiments.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an average of $1.5M per year for 5 years, supporting no more than 6 funded faculty researchers. Exceptions warranted by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

- For Topic 22, proposals are invited that include participation from Australian (AU) academic institutions; however, AU participation is not a requirement. In the case of proposals with AU participation, there still should be a single US primary institution and one PI submitting the overall proposal. Funding for the AU participation will be allocated separately by the AU government. Opportunities for Australian funding for such collaborative proposals are described at http://www.business.gov.au/ausmuri

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Topic 23 (ONR): Enhancing Thermal Transport at Material Interfaces

Background: The development of wide bandgap (WBG) semiconductor devices has led to unprecedented advancement of electronics that operate at high power and high frequency. However, the performance and reliability of these systems relies on the ability to efficiently dissipate thermal energy from the devices during operation. Although high thermal conductivity materials (e.g., diamond) have been used as heat spreaders in such devices, it has been found that the largest thermal resistance often

occurs at interfaces within the WBG device architecture, limiting the effectiveness of such solutions. While advances in first principle calculations have allowed for new insight into thermal processes in crystals, there still remains a lack of quantitative understanding of the underlying processes involved at interfaces. A number of models exist, but they frequently fail both quantitatively and qualitatively. New techniques such as modal analysis of molecular dynamics and non-equilibrium Green's function show promise for improved understanding of thermal transport at interfaces. At the same time, new optical techniques such as time-domain thermoreflectance have allowed for unprecedented measure of thermal conductance and boundary resistance.

Improved understanding of these processes will be used to guide the development of approaches to minimize thermal boundary resistance (TBR) in WBG devices. For example, it has been found that diffusive scattering in the interfacial region can either increase or decrease the thermal resistance. In addition, the patterning of material interfaces has been shown to enhance thermal transport at interfaces, resulting in a reduction of TBR by as much as 50%. By exploiting insights derived from the new theoretical formalisms, it may be possible to significantly reduce TBR opening up new WBG device architectures.

Objective: The objective of this MURI topic is the development of a rational method for designing thermal interfaces in wide bandgap electronic devices with extremely low thermal boundary resistance. A multidisciplinary research team will incorporate expertise in physics, materials science, electrical engineering and mechanical engineering to design, synthesize, characterize, and understand these materials. The impact of this approach will be the development of new high power and high frequency devices with reduced junction temperatures for RF, power, and optoelectronic applications.

Research Concentration Areas: Suggested research areas include but are not limited to: (1) Theoretical studies powered by advanced atomistic level simulations to quantify interfacial thermal processes; (2) Use of these theories to understand the role of anharmonicity, defects, roughness, and interdiffusion on thermal boundary resistance and to guide the design of patterned materials to enhanced thermal interfaces; (3) Growth of heteroepitaxial materials with controlled and patterned interfaces to demonstrate enhanced thermal interfaces; (4) Development of improved experimental tools to yield high accuracy measurements of structure, thermal transport and stability of these interfaces.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an average of $1.5M per year for 5 years, supporting no more than 6 funded faculty researchers.

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Topic 24 (ONR):   Self-Assessment of Proficiency for Autonomous and Intelligent Systems
Background: A significant shortcoming of autonomous and intelligent systems is their inability to recognize and understand how well they are (or could be) performing at a given task. Proficiency is a measure of an agent's achievable performance over the full range of operating parameters (e.g., parameters regarding environment, context, system, and task). Proficiency self-assessment is a foundational ability that agents must possess in order to operate successfully in dynamic, uncertain, and unstructured environments. Humans are adept at effective and continuous self-assessment and are generally accurate when it concerns assessing their own proficiency despite well-studied cognitive biases. Nevertheless, there is a substantial lack of detailed cognitive theories and corresponding computational models that address proficiency self-assessment. This shortfall persists not only when extrapolating to new or less-familiar tasks but also for familiar well-practiced tasks where performance is well known for certain values of operating parameters. For machines, significant research has occurred in recognition of known fault types and introspection for self-diagnosis. However, this work does not extend to non-fault situations where the primary factors affecting proficiency are operations

beyond prior experience and training data (i.e., poorly characterized regions of the operating parameter space). Related to proficiency self-assessment, there has been substantial recent and relevant progress in the fields of Machine Learning, Information Theory, and Artificial Intelligence (e.g., Bayesian and generative inference, active learning, metacognitive architectures, etc.). However, significant gaps remain as these approaches either operate on the output of the learning system or are part of learning system itself. This results in proficiency assessment approaches that are restricted to only the input information intended for the learning system and that afford the chance to inherit the learning system's brittleness. Other approaches assume non-trivial measures of performance have already been constituted or are ad hoc and lack a principled understanding or unifying theory of how to holistically approach proficiency self-assessment.

Objective: To develop methods and principles whereby intelligent and autonomous systems can assess their own proficiency based on knowledge of the task, environment, context, and system. The assessment methods should enable proficiency self-assessment i) a priori using only estimates of the environment, context, and potential states of the world, ii) in situ during task execution, and iii) ex post using knowledge of completed task. The range of tasks under consideration is broad and incorporates embodied / mobile systems and non-embodied / sensing systems (e.g., action selection, perception / recognition, world modeling, etc.).

Research Concentration Areas: 1) Underlying theory and principled approaches for proficiency self-assessment taking into account all available information and not restricted to only knowledge of the output of the autonomous system. Adaptation to improve proficiency is out of scope. 2) Computational models of proficiency self-assessment in humans across different levels of skill acquisition. These span the early, more conscious, and controlled level of cognitive processing to levels where these operations become increasingly automated, versatile, and decreasingly open to conscious awareness. 3) Metrics and principled methods to quantify proficiency and understanding how machines should measure, articulate to, and communicate their proficiency with humans to take advantage of the complimentary abilities of humans and machines.

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