ONR BAA Announcement Number: ONRBAA12-020



BROAD AGENCY ANNOUNCEMENT (BAA)

Fiscal Year (FY) 2013 Department of Defense Multidisciplinary Research Program of the

University Research Initiative

INTRODUCTION:

This publication constitutes a Broad Agency Announcement (BAA) as contemplated in Department of Defense Grant and Agreement Regulation (DODGARS) 22.315(a). A formal Request for Proposals (RFP), solicitation, and/or additional information regarding this announcement will not be issued. Request for the same will be disregarded.

The Office of Naval Research (ONR) will not issue paper copies of this announcement. The ONR and Department of Defense (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 ONR and other participating 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 BAA will not be returned. It is the policy of ONR and the other participating DoD Services to treat all proposals as sensitive competitive information and to disclose their contents only for the purposes of evaluation.

The DoD Multidisciplinary University Research Initiative (MURI), one element of the University Research Initiative (URI), is sponsored by the DoD research offices: 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").

Awards will take the form of grants. Therefore, proposals submitted as a result of this announcement will fall under the purview of the Department of Defense Grant and Agreement Regulations (DoDGARs).

NOTICE: Significant changes in funding and researcher team sizes have been made in this BAA. Please review carefully, in order to ensure that MURI projects under each topic are appropriately funded and that the size of research teams allows adequate funding for each faculty member to effectively contribute to exploring the scientific opportunities in the topic area, **EACH** MURI topic description will identify the topic chief's estimation of the anticipated funding available and the appropriate team size. Any requested exceptions should be discussed with the topic chief during

the white paper phase of the solicitation. The adequacy of support for each researcher will be an evaluation criterion in the source selection process.

Potential offerors may obtain information on ONR programs and opportunities by checking the ONR website at http://www.onr.navy.mil/en/Contracts-Grants/Funding-Opportunities/Broad-Agency-Announcements.aspx.

I. <u>GENERAL INFORMATION</u>

1. Agency Name

Office of Naval Research 875 North Randolph Street - Suite 1425 Code 03R Arlington, VA 22203-1995

2. Research Opportunity Title

Multidisciplinary University Research Initiative (MURI)

3. Program Name

Fiscal Year (FY) 2013 Department of Defense Multidisciplinary Research Program of the University Research Initiative

4. Research Opportunity Number

ONRBAA12-020

5. Response Date

White Papers: 09 October 2012

Full Proposals: 10 December 2012

6. 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 interact to provide rapid advances in scientific areas of interest to the DoD. As defined by the DoD, "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." (http://comptroller.defense.gov/fmr/02b/02b_05.pdf). The DoD's basic research program invests broadly in many specific fields to ensure that it has early cognizance of new scientific knowledge.

The FY 2013 MURI competition is for the topics listed below. Detailed descriptions of the topics can be found in Section VIII entitled, "Specific MURI Topics", of this BAA. The detailed descriptions are intended to provide the proposer 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 full proposals addressing the following topics 1 through 8 should be submitted to the Army Research Office (ARO):

- 1. Artificial Cells for Novel Synthetic Biology Chassis
- 2. Molecular Co-Crystal Design and Synthesis
- 3. Reduced Cyber-system Signature Observability by Intelligent and Stochastic Adaptation
- 4. Non-equilibrium Many-body Dynamics
- 5. Materials with Spin Mediated Thermal Properties
- 6. Transforming Information within Nonequilibrium Nanosystems
- 7. Controlling Collective Phenomena in Complex Networks
- 8. Physiochemical Determinants of Cognition and Decision Making

White papers and Full proposals addressing the following topics 9 through 15 should be submitted to the Air Force Office of Scientific Research (AFOSR):

9. Measurement and Verification Methods in Quantum Information Science

- 10. New Quantum Phases of Matter
- 11. Multiphysics and Multiscale Failure Prediction through Peridynamic Theory
- 12. Electrochemical Dynamics in Nanoscale Systems
- 13. A New Paradigm in Sources and Physics of High-Power Ionospheric Modification
- 14. Magneto-electric Energy Conversion Materials: Terahertz Emission and Efficient Energy Conversion in Unbiased Dielectrics
- 15. Photonic Synthetic Matter

White papers and full proposals addressing the following topics 16 through 23 should be submitted to The Office of Naval Research:

- 16. Random Lasers, Nano-spasers and Optical Rogue Waves
- 17. Free Space Optical Quantum Key Distribution (QKD)
- 18. Integrated Nanophotonics
- 19. Exploitation of Natural and Anthropogenic Noise for Ocean Exploration
- 20. Rare Element Replacement Strategies
- 21. Acoustic Metamaterials
- 22. Cognitive Neuroscience of Memory Consolidation across Sleep Stages and Efficient Learning
- 23. Computational Foundations of Moral Cognition

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.

7. Point(s) of Contact

One or more Research Topic Chiefs are identified for each specific MURI Topic. Questions of a technical nature shall be directed to one of the Research Topic Chiefs identified in Section VIII entitled, "Specific MURI Topics" of this BAA.

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. Bill Lukens MURI Program Manager Office of Naval Research, Code 03R E-mail Address: william.lukens1@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 the cognizant Contract Specialist, as specified below:

Primary: Jennifer Brown Contract and Grants Awards Management, Code ONR 0251 Office of Naval Research 875 North Randolph Street, Suite W1272F Arlington, VA 22203-1995 E-Mail: jennifer.brown4@navy.mil

Secondary: Vera M. Carroll Acquisition Branch Head Contract and Grants Awards Management, Code 0251 Office of Naval Research 875 North Randolph Street, Suite 1279 Arlington VA, 22203-1995 E-mail: vera.carroll@navy.mil

Questions submitted within 2 weeks prior to a deadline may not be answered, and the due date for submission of the white paper and/or full proposal will not be extended. Answers to questions submitted in response to this BAA will be addressed in the form of an Amendment and will be posted to one or more of the following webpages:

- Grants.gov Webpage http://www.grants.gov/
- ONR Broad Agency Announcement (BAA) Webpage http://www.onr.navy.mil/en/Contracts-Grants/Funding-Opportunities/Broad-Agency-Announcements.aspx

8. Instrument Type(s)

It is anticipated that all awards resulting from this announcement will be grants.

9. Catalog of Federal Domestic Assistance (CFDA) Numbers

12.300 ONR 12.800 AFOSR 12.431 ARO

10. Catalog of Federal Domestic Assistance (CFDA) Titles

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

11. Other Information

The Non-ONR Agency Information:

Air Force Office of Scientific Research 875 North Randolph Street Suite 325 Room 3112 Arlington, VA 22203-1768

> Army Research Office 4300 S. Miami Blvd. Durham, NC 27703-9142

Work funded under this BAA must be basic research and falls under the guidance of the Under Secretary of Defense (Acquisition, Technology, and Logistics) Memorandum of 24 MAY 2010.

II. AWARD INFORMATION

It is anticipated 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 2-year option period to bring the total maximum term of the award to five years. The base and option period will be incrementally funded.

Total amount of funding for five years available for grants resulting from this MURI BAA is estimated to be about \$250 million dollars pending out-year appropriations. MURI awards are \$1M- \$2.5M per year, with the actual amount contingent on availability of funds, the specific topic, and the scope of the proposed work. Typical annual funding is in the \$1.25M to \$1.5M range. The amount of the award and the number of supported researchers may not exceed the

limit the limit specified for the individual topics in Section VII. It is strongly recommended that potential proposers communicate with the Program Topic Chief 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

This MURI competition is open only to and full 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 an FFRDC, a University Affiliated Research Center (UARC) or other University Affiliated Laboratory (UAL) is eligible to submit a proposal to this MURI competition and receive MURI funds. However, the eligibility of a UAL (other than an FFRDC) to submit a URI proposal does not exempt the proposal from any evaluation factor contained in this Broad Agency Announcement. Ineligible organizations (e.g., industry, DoD laboratories, Federally Funded Research and Development Centers (FFRDCs), and foreign universities) may collaborate on the research but may not receive MURI funds, directly or via subaward.

When a modest amount of additional funding for an ineligible organization is necessary to make the proposed collaboration possible, such funds may be requested via a separate proposal from that organization. This supplemental proposal should be attached to the primary MURI proposal and will be evaluated separately by the responsible Research Topic Chief. If approved, the supplemental proposal will be funded by the responsible agency using non-MURI funds. Since it is not certain that non-MURI funding would be available for ineligible organizations, Principal Investigators are encouraged to restrict funding requests to eligible organizations when practical.

Awards under this BAA will be made only to U.S. Institutions of Higher Education which award degrees in science and/or engineering. Historically Black Colleges and Universities (HBCUs) and Minority Institutions (MIs) are encouraged to submit proposals and join others in submitting proposals. However, no portion of this BAA will be set aside for HBCU and MI participation.

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 170.110. Any company, non-profit agency or university that applies for financial assistance (either grants, cooperative agreements or other transaction agreements) as either a prime or sub-recipient under this BAA 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 170.220. An entity is **exempt** from this requirement **UNLESS** in the preceding fiscal year it received: a) 80 percent or more of its annual gross revenue in Federal contracts (and subcontracts), loans, grants (and subgrants), and cooperative agreements; b) \$25 million or more in annual gross revenue from Federal contracts (and subcontracts), loans, grants (and subgrants), and cooperative agreements; b) \$25 million or 15(d) of the Securities Exchange Act of 1934 or section 6104 of the Internal Revenue Code of 1986.

IV. APPLICATION AND SUBMISSION INFORMATION

1. Application and Submission Process

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 full 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 full proposals. The Topic Chief may also on occasion provide feedback encouraging reteaming to strengthen a proposal.

<u>Due Date</u>: The due date and time for receipt of white papers is no later than 4:00 P.M. (Eastern Time) on Tuesday, 09 October 2012.

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 at the agency specified for the topic. For hard copy submissions, use the addresses provided in Section IV entitled, "Application and Submission Information" paragraph number 6 entitled, "Address for the 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.

<u>Evaluation/Notification</u>: Initial evaluations of the white papers will be issued on or about Monday, 22 October 2012.

Submission of Full Proposal:

Any Offeror may submit a full proposal even if its white paper was not identified as being of "particular value" to the Government. However, the initial evaluation of the white papers should give prospective awardee some indication of whether a later full proposal would likely result in an award.

NOTE: Full Proposals must be submitted electronically through grants.gov.

Registration Requirements for Grants.gov: There are several one-time actions you must complete in order to submit an application through Grants.gov (e.g., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the Central Contract Registry (CCR), register with the credential provider, and register with Grants.gov). See <u>www.grants.gov/GetStarted</u> to begin this process. Use the Grants.gov Organization Registration Checklist at <u>www.grants.gov/assets/OrganizationRegCheck.doc</u> to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at <u>least 21 days</u> completing these requirements. It is suggested that the process be started as soon as possible.

Questions: 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 or support@grants.gov.

2. Content and Format of White Papers and Full Proposals

The white papers and full proposals submitted under this BAA are expected to address unclassified basic research. White papers and full proposal submissions will be protected from unauthorized disclosure in accordance with applicable law and DoD regulations. Proposers are expected to appropriately mark each page of their submission that contains proprietary information. Grants awarded under this announcement shall be unclassified.

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

a. White Paper Submission: Contents and Format of Applications

Each topic in this announcement has one or more Research Topic Chiefs identified from one of the participating agencies; ONR, AFOSR, or ARO. You should submit your white paper to one of the Research Topic Chiefs at the agency for which you are applying.

White paper format should 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, and curriculum vitae). White paper pages beyond the 4-page limit may not be evaluate or read.

White Paper content should be as follows:

- A one page cover letter (optional)
- A cover page, labeled "PROPOSAL WHITE PAPER," that includes the BAA 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

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.

Copies – one (1) original and two (2) copies.

b. Grants.gov Full Proposal Submission: Content and Format of Applications

Application forms and instructions are available at Grants.gov. To access these materials, go to <u>http://www.grants.gov</u>, select "Apply for Grants", and then select "Download Application Package". Enter the CFDA for the respective agency to which you are directing the application (ONR – 12.300, AFOSR – 12.800, ARO – 12.431), as found on page five of this announcement) and the funding opportunity number, designated as "research opportunity number" on page two of this announcement. Each topic in this announcement has a Research Topic Chief identified from one of the participating agencies; ONR, AFOSR, or ARO. You should direct your application to the agency associated with the topic for which you are applying.

Content and Form of Application – SF 424 (R&R) - Mandatory

You must complete the mandatory forms in accordance with the instructions 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 this form first to populate data in other forms. 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). To be considered for award, applicants must fill out block 4 of the SF 424 R&R as follows: Block 4a "Federal Identifier": leave blank; Block 4b "Agency Routing Identifier": enter the appropriate topic chief's name.

Form Research & Related Other Project Information - Mandatory

Complete questions 1 through 6 and attach files. The files must comply with the following instructions:

Project Summary/Abstract (Field 7 on the Form) - Mandatory

The project summary should be a single page that identifies 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 and the total funds requested from DoD for the 3-year base period, the 2-year option period and the 5-year total period. The project summary must not exceed 1 page when printed using standard 8.5" by 11" paper with 1" margins (top, bottom, left and right) with font Times New Roman 12 point. To attach a Project Summary/Abstract, click "Add Attachment."

Project Narrative (Field 8 on the form) - Mandatory

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 - no more than twenty-five (25) single-sided pages. The cover, table of contents, list of references, letters of support, and curriculum vitae are excluded from the page limitations. Full proposals exceeding the page limit may not be evaluated.

Include the Following in Field 8

The first page of your narrative must include the following information:

- Principal Investigator name
- Phone number, fax number and e-mail address
- Institution, Department, Division
- Institution address
- Other universities involved in the MURI team
- 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
- <u>Table of Contents</u>: List project narrative sections and corresponding page numbers.
- <u>Technical Approach</u>: 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 full time equivalent graduate students and undergraduates, if any, to be supported each year. Discuss the involvement of other students, if any.
- <u>Project Schedule, Milestones and Deliverables</u>: A summary of the schedule of events, milestones, and a detailed description of the results and products to be delivered.
- <u>Management Approach</u>: 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.

(a) 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, by version and/or configuration that are required for the proposed effort.

(b) 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.

(c) 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 Program Topic Chief. Briefly summarize the qualifications of the Principal Investigator and other key investigators to conduct the proposed research.

(d) List the amount of funding and describe the research activities of the Principal Investigator and co-investigators in on-going and pending research projects, whether or not acting as Principal Investigator in these other projects, the time charged to each of these projects, and their relationship to the proposed effort.

(e) Describe plans to manage the interactions among members of the proposed research team.

(f) 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.
- <u>Letters of Support</u>: Up to three Letters of Support from various DoD agencies may be included.
- <u>Curriculum Vitae</u>: Include curriculum vitae of the Principal Investigator and key co-investigators.

All applications should be in a single PDF file. To attach a Project Narrative in Field 8, click "Add Attachment."

Bibliography & References Cited (Field 9 on the form)

Facilities & Other Resources (Field 10 on the form)

Equipment (Field 11 on the form)

Other Attachment (Field 12 on the form)

Attach budget proposal at field 12. You 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. The option must be separately priced. The Research and Related Budget form is not required.

The budget should 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 July 2013. For the three-year base grant, the cost should be broken down to reflect funding increment periods of:

- (1) Three months,
- (2) Twelve months,
- (3) Twelve months and
- (4) Nine 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) Three months
- (2) Twelve months, and
- (3) Nine months.

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

• <u>Direct Labor</u> – Individual labor categories or persons, with associated labor hours and unburdened direct labor rates. Provide 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.

• <u>Fringe Benefits and Indirect Costs</u> (i.e., 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.

• <u>Travel</u> – 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.

<u>Subawards</u> – Provide a description of the work to be performed by the subrecipients. For each subaward, a detailed cost proposal is required to be included in the principal investigator's cost proposal. Fee/profit is unallowable.
<u>Consultants</u> – 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 contractor's proposal.

• <u>Materials & Supplies</u> – Provide an itemized list of all proposed materials and supplies including quantities, unit prices, proposed vendors (if known), 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, office equipment and furnishings, etc.) 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.

• <u>Other Direct Costs</u> – Provide an itemized list of all other 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).

<u>NOTE</u>: If the grant proposal is for a conference, workshop, or symposium, the proposal should include the following statement: "The funds provided by ONR will not be used for food or beverages." • Fee/Profit – Fee/profit is unallowable.

Funding Breakdown

Funding breakdown corresponding to the proposed Technical Approach which was provided in Field 8 of the Research and Related Other Project Information Form must also be attached.

Proposal Receipt Notices

After a full 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 <u>watch</u> for and <u>save</u> each of the e-mails. You will know that your proposal has reached ONR, ARO or AFOSR when the AOR receives e-mail Number 3. You will need the Submission Receipt Number (e-mail Number 1) to track a submission. The three e-mails are:

Number 1 – The applicant will receive a confirmation page upon completing the submission to Grants.gov.

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.)

Number 3 – The third notice is an acknowledgment of receipt in e-mail form from the designated agency within ten days from the proposal due date. The e-mail is sent to the authorized

representative for the institution. The e-mail for proposals notes that the proposal has been received and provides the assigned tracking number.

3. Significant Dates and Times

Schedule of Events		
Event	Date	Time
Questions Regarding white papers	25 September 2012 *	2:00PM Eastern Daylight Time
White Papers Due	09 October 2012	4:00 PM Eastern Daylight Time
Notification of Initial DoD Evaluations of White Papers	22 October 2012	
Questions Regarding full proposals	26 November 2012 *	2:00PM Eastern Standard Time
Full Proposals Due	10 December 2012	4:00 PM Eastern Standard Time
Notification of Selection for Award	8 April 2013 **	
Start Date of Grant	1 July 2013 **	

*Questions received after this date and time may not be answered, and the due date for submission of the proposals 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 the Office of Naval Research 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 proposal should be submitted long enough before the deadline established in the solicitation so that it will not be received late and thus be ineligible for award consideration.

4. Submission of Late Proposals

Any full proposal submitted and validated through Grants.gov where the time and date for submission (e-mail Number #2) is after the deadline for proposal submission in Section IV entitled, "Application and Submission Information" paragraph number 3 entitled, "Significant Dates and Times" will be late and will not be evaluated unless the Grants.gov website was not operational on the due date and was unable to receive the proposal submission. If this occurs, the time specified for the receipt of proposals through Grants.gov will be extended to the same time of the day specified in this BAA on the first workday on which the Grants.gov website is operational.

Be advised that Grants.gov applicants have been experiencing system slowness and

validation issues which may impact the time required submitting proposals. 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 soft-copy proposals be uploaded at least two days before the deadline established in the solicitation so that it will not be received late and be ineligible for award consideration.

a. For ARO, use the following alternative to submitting proposals to grants.gov.

Email your completed proposal package and grants.gov trouble ticket/case number to aror.baa@us.army.mil. Your proposal must include all signatures and attachments and be submitted in PDF format. All proposal submissions will be subsequently evaluated by ARO for completeness and an official email confirmation will be sent. Incomplete packages will not be considered for an award. All submissions must meet the deadline for full proposals specified in the BAA.

b. For AFOSR submissions please email your completed proposal package and grants.gov trouble ticket/case number to proposal@afosr.af.mil. Each email may not exceed 35MB. If necessary, use multiple emails sending the full proposal noting the trouble ticket/case number. Your proposal must include all signatures and attachments and be submitted in PDF format. An auto-reply email will be returned to the sender indicating that your email arrived. All proposal submissions will be subsequently evaluated by AFOSR for completeness and an official email confirmation will be sent. Incomplete packages will not be considered for an award. All submissions must meet the deadline for full proposals specified in the BAA.

c. There is no alternative process for ONR. Full proposals must be submitted through grants.gov.

5. 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 Offeror 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 (ordinary First Class or Priority Mail (but not Express Mail)):

U.S. Army Research Office (FY12 MURI) P. O. Box 12211 Research Triangle Park, NC 27709-2211

For commercial delivery (such as Express Mail, FedEx, UPS, etc.):

U.S. Army Research Office (FY12 MURI) For white papers include: ATTN: (list name of responsible Research Topic Chief) 4300 S. Miami Blvd Durham, NC 27703-9142 919-549-4211

Air Force Office of Scientific Research:

Hard copy white papers addressing topics (9) to (15) 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

Office of Naval Research:

Hard copies of white papers topics (16) to (23) 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. William Lukens

Email: William.lukens1@navy.mil 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.

NOTE: White Papers sent by fax or hand delivered will not be considered.

V. EVALUATION INFORMATION

1. Evaluation Criteria

A. Basic Research: The MURI Program is funded by basic research (Budget Activity 1) money. White papers and full 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 requirements." The full definitions of these terms are contained in the links http://comptroller.defense.gov/fmr/02b/02b_05.pdf

White papers will be evaluated by the responsible Research Topic Chief 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 full proposal. The assessment will focus on scientific and technical merits (criterion 1, below), potential for the research to significantly advance fundamental understanding in the topic area (criterion 2 below), and potential DoD interest (criterion 3, below), although the other criteria may also be used in making the assessment.

Full proposals responding to this BAA in each topic area will be evaluated using the following criteria. The first four evaluation factors are of equal importance:

(1) Scientific and technical merits of the proposed basic science and/or engineering research;

(2) Potential for the research, if successful, to significantly advance fundamental understanding in the topic area;

- (3) DoD potential interest in the proposed research; and
- (4) qualifications and availability of the Principal Investigator and other investigators

The following three evaluation criteria are each of lesser importance than any of the above four, but are equal to each other:

(5) adequacy of current or planned facilities and equipment to accomplish the research objectives;

(6) 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

(7) realism and reasonableness of cost (cost sharing is not a factor in the evaluation).

Decisions for exercising options will be based on accomplishments during the base years and potential research advances during the option years that can impact DoD research priorities and technological capabilities.

2. Evaluation Panel

White papers 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 specialized government employees secured under the Intergovernmental Personnel Act (IPA). These individuals will sign a conflict of interest statement prior to receiving proposal information.

Full proposals will undergo a multi-stage evaluation procedure. The cognizant Program Officer 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 peers from the university community may be utilized as subject-matter-expert technical consultants. Similarly, support contractors may be utilized to evaluate cost proposals. However, proposal selection and award decisions are solely the responsibility of Government personnel. Each support contractor's employee and peer from the university community having access to technical and cost proposals submitted in response to this BAA will be required to sign a non-disclosure 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 by the Principal Investigator and the government prior to final award.

VI. AWARD ADMINISTRATION INFORMATION

1. Administrative Requirements –

Central Contractor Registration: All Offerors submitting proposals or applications must:

- (a) be registered in the Central Contractor Registration (CCR) prior to submission;
- (b) maintain an active CCR registration with current information at all times during which it has an active Federal award or an application under consideration by any agency; and
- (c) provide its DUNS number in each application or proposal it submits to the agency.

2. Reporting

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

VII. OTHER INFORMATION

1. Government Property/Government Furnished Equipment (GFE) and Facilities

Government research facilities and operational military units are available and should be considered as potential government-furnished equipment/facilities. These facilities and resources are of high value and some are in constant demand by multiple programs. It is unlikely that all facilities would be used for any one specific program. The use of these facilities and resources will be negotiated as the program unfolds. Offerors should explain as part of their proposals which of these facilities are critical for the project's success.

2. Use of Animals and Human Subjects in Research

If animals are to be utilized in the research effort proposed, the Offeror must complete a DoD Animal Use Protocol with supporting documentation (copies of AAALAC accreditation and/or NIH assurance, IACUC approval, research literature database searches, and the two most recent USDA inspection reports) prior to award. For assistance with submission of animal research related documents, contact the ONR Animal Use Administrator at (703) 696-4046.

Similarly, for any proposal for research involving human subjects, the Offeror must submit or indicate an intention to submit prior to award: documentation of approval from an Institutional Review Board (IRB); IRB-approved research protocol; IRB-approved informed consent form; proof of completed human research training (e.g., training certificate or institutional verification of training); an application for a DoD-Navy Addendum to the Offeror's DHHS-issued Federal wide Assurance (FWA) or the Offeror's DoD-Navy Addendum. In the event that an exemption criterion under 32 CFR.219.101 (b) is claimed, provide documentation of the determination by the Institutional Review Board (IRB) Chair, IRB vice Chair, designated IRB administrator or official of the human research protection program including the category of exemption and short rationale statement. This documentation must be submitted to the ONR Human Research Protection Official (HRPO), by way of the ONR Program Officer. Information about assurance applications and forms can be obtained by contacting ONR_343_contact@navy.mil. If the research is determined by the IRB to be greater than minimal risk, the Offeror also must provide the name and contact information for the independent medical monitor. For assistance with submission of human subject research related documentation, contact the ONR Human Research Protection Official at (703) 696-4046.

For contracts and orders, the award and execution of the contract, order, or modification to an existing contract or order serves as notification from the Contracting Officer to the Contractor that the HRPO has approved the assurance as appropriate for the research under the Statement of Work and also that the HRPO has reviewed the protocol and accepted the IRB approval or exemption determination for compliance with the DoD Component policies. See, DFARS 252.235-7004.

3. Recombinant DNA

Proposals which call for experiments using recombinant DNA must include documentation of compliance with Department of Human and Health Services (DHHS) recombinant DNA regulations, approval of the Institutional Biosafety Committee (IBC), and copies of the DHHS Approval of the IBC letter.

4. Department of Defense High Performance Computing Program

The DoD High Performance Computing Program (HPCMP) furnishes the DoD S & T and DT & E communities with use-access to very powerful high performance computing systems. Awardees of DoD contracts, grants, and assistance instruments may be eligible to use HPCMP assets in support of their funded activities if 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/.

5. Project Meetings and Reviews

Generally an annual program review will be required by the DoD program manager. Other reviews will be held as necessary. Program status reviews are 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, offerors should assume that 40% of these meetings will be at or near ONR, Arlington, VA and 60% at other contractor or government facilities. Interim meetings are likely, but if possible these will be accomplished via video telephone conferences, telephone conferences, or via web-based collaboration tools.

6. Other Guidance, Instructions and Information

None

VIII. SPECIFIC MURI TOPICS

ARO FY2013 MURI TOPIC #1

Submit white papers and proposal to Army Research Office

Artificial Cells for Novel Synthetic Biology Chassis

Background: The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-celled organisms (e.g., bacteria, yeast) are typically used as synthetic biology chassis, the complexity of these relatively simple organisms presents challenges for achieving robust and predictable engineered systems. Endogenous cellular regulatory systems often interfere with the function of synthetic biological elements, and biomolecules can diffuse throughout the cellular compartment in which they reside, interacting with any suitable binding partners.

A potential solution to this challenge is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Recent advances toward minimal biological cells have demonstrated basic biological processes within simple lipid vesicles that require several enzymatic steps, including protein expression and DNA replication. In addition, advances in computational modeling now enable the modular design and simulation of large scale synthetic biology systems containing thousands of compartments and hundreds of reactions and species per compartment. While minimal cells would provide a simplified synthetic biology chassis, these fully biological systems still suffer from complexity, unpredictability and a lack of robustness. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, responsive nanoscale cages, and composite microparticles with stable internal compartments. There is currently an opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that combines for the first time the specificity and complexity of biology with the stability and control of synthetic chemistry and materials science.

Objective: The objective of this MURI is to understand the integration of biological and biomimetic synthetic cellular elements to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways. These hybrid biological/synthetic cells will provide a fundamentally new chassis for synthetic biology that addresses the critical challenge of instilling increased control and stability to engineered biological systems.

Research Concentration Areas: Suggested research areas include, but are not limited to the following: 1) Predictive modeling and comprehensive characterization of interactions between biological and synthetic elements in the context of a modular multi-compartment biological system. 2) Synthesis and characterization of internal structures and/or compartments that could organize components within the artificial cell. 3) Development of approaches to target/sequester biomolecules to synthetic intracellular structures and elucidation of the impact of sequestration/immobilization on biological activity. 4) Characterization of biological transport into and out of a hybrid biological/synthetic cell. 5) Evaluation of the potential to substitute natural building blocks (e.g., amino acids, lipids) with non-natural replacements to achieve new functions

and/or properties. 6) Comprehensive analysis of the activity and robustness of genetic circuits or biological pathways within a hybrid biological/synthetic cell.

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 six 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. Stephanie McElhinny, ARO, 919-549-4240, stephanie.a.mcelhinny.civ@mail.mil; Dr. Jennifer Becker, ARO, 919-549-4224, jennifer.j.becker.civ@mail.mil

ARO FY2013 MURI TOPIC #2

Submit white papers and proposal to Army Research Office

Molecular Co-Crystal Design and Synthesis

Background: The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Molecular cocrystals contain two or more neutral molecular components that rely on non-covalent interactions such as hydrogen bonding, π -stacking, and van der Waal's forces to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure 'parent' crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in chemistry and materials science research. A recent breakthrough discovery demonstrates that cocrystallization can be used to generate novel solid forms of energetic materials, and guite remarkably, energetic binary co-crystals of trinitrotoluene and 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) in a 1:1 mole ratio were obtained. The relevant properties of the resulting co-crystal are a decrease in sensitivity (factor of two relative to CL-20) while maintaining almost all of energy density relative to CL-20. The functionality of many energetic materials is limited to nitro-groups, and the dominant intermolecular forces offer few predictable interactions sufficiently strong or versatile to be useful in co-crystal design. Weak intermolecular forces (e.g., dispersion) are difficult to quantify using computational chemistry methodologies, and even more challenging is the prediction of crystal structure from molecular structure. Novel molecular co-crystals can also be designed and synthesized to obtain unprecedented properties in organic ferroelectric and organic nonlinear optical materials (NLO). Initial reports indicate that co-crystals of nonpolar (symmetric) organic molecules (phenazine and chloro- or bromo-anilic acid) exhibit non-centrosymmetric packing, and high room temperature dielectric constants. It is possible to tune the dielectric constants further by varying the composition, mole ratio, or by adding additional components to make ternary compounds. Similarly, molecular co-crystal approach is also shown to be very useful in tuning nonlinear optical properties of different organic materials.

Objective: The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties.

Research Concentration Areas: Research is sought that will lead to a new understanding of weak intermolecular forces and how such forces can be used for the design of novel molecular cocrystalline materials. Suggested research areas may include, but are not limited to the following: 1.) Development of new computational methods using quantum-based interactions such as SAPT(DFT) and others, for accurate co-crystal structure prediction to identify promising synthetic targets; 2.) Development of new, predictable supramolecular synthetic strategies, or synthons, with a focus on co-crystal assembly for new designs of energetic, organic ferroelectric (thin film or bulk), and NLO materials; 3.) Material characterization of co-crystals to determine composition, structure, and material performance, and 4.) Optimization of co-crystal physical and chemical properties through molecular refinement using computation and Material Science to identify new synthetic targets. **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 seven 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. James Parker, 919-549-4293, james.k.parker30.civ@mail.mil; Dr. Pani Varanasi, 919-549-4325, chakrapani.v.varanasi.civ@mail.mil

ARO FY2013 MURI TOPIC #3

Submit white papers and proposal to Army Research Office

Reduced Cyber-system Signature Observability by Intelligent and Stochastic Adaptation

Background: Leveraging recent advances in network science, game theory, and control theory, this topic seeks to create the theoretical underpinnings necessary for the creation of adaptive systems that are robust, resilient and survivable against cyber attacks. This new science will enable future information systems to be adaptive and exhibit non-deterministic characteristics to adversaries, making it extremely difficult and costly for them to be attacked, and guide the creation of adaptive defense strategies in response to changing threats and attacker behaviors. Current research on military MANETs where networks are forced to change in response to mobility provides the much-needed initial insight into adaptive systems with regards to resiliency and agility, but scientific foundations for proactive adaptive schemes are missing. In cyber defense, the unpredictable nature of human adversaries further complicates problem, making it extremely challenging to understand and model attack/defense dynamics. Fortunately, recent advances in adversarial reasoning (application of Stackleberg theory to adversarial games) provide a means to extract and analyze adversarial behaviors in a tractable way, necessary for the establishment of adaptive and proactive information systems for cyber defense. Another promising new research area aims at creating theoretical foundations for analyzing and modeling cyber-attack/defense under a control theory framework; one could consider that attackers and defenders have separate, but inter-related objective functions and "control loops". New insights from a control theory perspective, especially techniques for system analysis under adversarial settings, will enable one to define optimized defense strategies, and to create cyber systems that can maximize their availability, stability and functionality, while concomitantly minimizing their "observability" and "vulnerability" to minimize exploitation by their attackers.

Objectives: To establish scientific foundations of adaptive systems that are robust, resilient and survivable against cyber attacks and to create proactive multi-level cyber defense strategies that will minimize an attacker's ability to understand and to attack such systems.

Research Concentration Area: Suggested approaches may include, but are not limited to, collaborative work in computing and information sciences especially adversarial reasoning and game theory, network science, control theory, biology, mathematics and statistics that include 1) Analytical models and performance metrics capturing the dynamics between cyber-attack and defense; 2) Network science and a unified framework for analyzing resiliency, agility, and performance trade-offs, for both proactive cyber defense adaptation and reactive response to network mobility; 3) New models/principles from control theory that incorporate attack/defense dynamics under adversarial settings, for analyzing and assuring system robustness and resiliency and for guiding the creation of optimal defense strategies; 4) Under the cyber defense context, advances in game theory that deal with dynamic, non-linear, and non-cooperative players, and to reason with incomplete and imprecise adversarial information; 5) A new quantitative definition of system resiliency and robustness under an adversarial setting, with the incorporation of attack/response dynamics. (Current resiliency and robustness analysis frameworks are derived from reliability engineering theory, focusing mainly on natural failures); 6) Novel adaptive techniques based on active jamming, randomization and obfuscation for information protection, complementary to encryption at the bit and byte level; 7) Bio-inspired cyber defense techniques in cyber deception, adaptation, evolution, and self-regeneration.

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 eight 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. Cliff Wang, ARO, 919-549-4207, cliff.x.wang.civ@mail.mil

ARO FY2013 MURI TOPIC #4

Submit white papers and proposal to Army Research Office

Non-equilibrium many-body dynamics

Background: Dynamics far from equilibrium is of great importance across S&T, including in materials science, condensed-matter physics, nonlinear optics, chemistry, biology, biochemistry, and recently has taken on significance in atomic physics, where new tools will enable breakthroughs. In particular, optical lattice emulation is allowing one to gain insight, and potentially solve, traditionally intractable problems, including non-equilibrium. Breakthroughs in other disciplines are also enabling a new look at non-equilibrium. In materials science, a recent pumpprobe experiment enabled dynamical control of material properties [Science 317 769]. Another example is in biochemistry, in determining the role that non-equilibrium phase transitions play in driven biochemical networks, e.g., canonical phosphorylation - dephosporylation systems with feedback that exhibit bistability [J. R. Soc. 8,107, J Phys Chem B 110, 15063]. Despite the ubiquitous nature of non-equilibrium dynamics, making scientific progress has been difficult. One of the many challenges is finding many-body systems that remain far from equilibrium on experimentally accessible time scales. As mentioned, recent breakthroughs in materials science, nonlinear optics [Nat Phys 3 807, Science 320 769, Rep Prog Phys 68 1129], cold atoms in lattices, and biochemistry, now offer scientific opportunities to explore these systems and to develop theoretical understanding. Currently, science lacks understanding of even the most basic questions. Is there universality in non-equilibrium dynamics? Is there emergent collective behavior which would allow for the classification of all (or most) dynamics into several fundamental categories? When do isolated systems thermalize from non-equilibrium initial states? What conditions indicate or are required for such equilibration? How do guasiparticle excitations and/or entanglement propagate in "guenched" systems, i.e., when there is a sudden change of the system parameters? Are there ways to engineer systems, e.g., using dissipation, such that they lead to robust designed (e.g., highly correlated) states. How do classical and quantum nonequilibrium phenomena differ? Answering these questions will open new scientific and technological opportunities in numerous disciplines.

Objective: Discover how many-body systems thermalize from non-equilibrium initial states, and explore the dynamics of far-from-equilibrium systems. As examples explore (1) non-equilibrium phase transition such as in driven biochemical networks, in an effort to identify how to obtain specific biochemical functions; (2) dynamic control of materials properties, e.g., photo-induced phase transitions; (3) rapid quenching, to evaluate the propagation of quasiparticle excitations and entanglement; and (4) feedback and measurement in quantum many-body systems, including engineering dissipative quantum systems that evolve to highly-correlated quantum states.

Research Concentration Areas: Possibilities include, but are not limited to the following: developing experimental manifestations of non-equilibrium dynamics under controllable conditions (such as in optical lattices or other systems); modeling of complex systems such as biochemical reactions; exploring dynamic control of materials (e.g., photo-induced phase transitions or phosphorylation with feedback); theoretical treatments of quantum many-body dynamics far from equilibrium; exploitation of nonlinear optics, nonlinear and stochastic mathematics, quantum information and control.

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 seven 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. Paul Baker, ARO, 919-549-4202, <u>paul.m.baker4.civ@mail.mil</u>; Dr. Marc Ulrich, ARO, 919-549-4319, <u>marc.d.ulrich.civ@mail.mil</u>

ARO FY2013 MURI TOPIC #5

Submit white papers and proposal to Army Research Office

Materials with Spin Mediated Thermal Properties

Background: The emerging research area of materials with spin mediated thermal properties offers unique opportunities for breakthrough research in physics and materials science. Recent extraordinary observations of the spin-Seebeck effect in ferromagnetic materials (NiFe) followed by semiconductors (GaMnAs) and insulators (LaY₂Fe₅O₁₂), as well as the magnon thermal Hall effect in ferromagnetic insulator materials (Lu₂V₂O₇), indicate exciting opportunities for the discovery of other novel materials with unprecedented spin-caloritronic properties. In addition, recent findings also indicate extraordinary ballistic spin thermal transport phenomena in spin-chain compounds (SrCuO₂). It has recently been shown that it is possible to achieve high thermal conductivity of 100 W/m-K at room temperature in La₅Ca₉Cu₂₄O₄₁spin-ladder compounds. Tunable thermal conductivity (with magnetic field) in materials was also demonstrated in some materials such as $K_2V_3O_8$ expanding the exciting research opportunities in the area of spin mediated thermal properties of materials. Although thermal conductivity due to magnons has been observed in materials (mostly limited to low temperatures), little progress has been made to understand the mechanisms of interactions (such as magnon-magnon, magnon-phonon, magnondefects etc.) that influence mean free paths of spin waves in these materials. This knowledge is essential to synthesize materials with high thermal conductivity above room temperatures. Thermal transport by phonons and electrons in materials is well studied but relatively little is known about the heat transport in materials by spin excitations (i.e. thermal conductivity by magnons). Fundamental understanding of the magnon interactions would accelerate synthesis of novel materials with unprecedented thermal conductivity properties. Similarly, understanding the mechanisms responsible for the experimentally observed Spin Seebeck effect in materials could help to design novel materials with enhanced figure of merit.

Objective: The objective is to demonstrate novel materials and structures with extraordinary thermal properties mediated by electronic spin. Successful proposals will establish the basic physics of magnon interactions, the Spin Seebeck effect, etc. observed in materials as well as composition-processing-structure -property relationships in these complex materials.

Research Concentration Areas: Research areas may include, but are not limited to the following: 1) Advance comprehensive theories (such as phonon-drag mechanism for the spin-Seebeck effect, influence of magnon interactions on the thermal conductivity in materials etc.) to elucidate mechanisms for spin mediated thermal properties of materials. 2) Develop novel characterization techniques to enhance understanding and verify theories of quantum interactions in spin-chain and ladder compounds and the Spin Seebeck effect observed in various materials. 3) Systematic experimental studies to identify mechanisms that limit mean free paths of spin waves in spin-chain, ladder materials and then grow high quality single crystals and thin films of novel materials with enhanced thermal conductivity. 4) Based on the theory and using predictive models, design and synthesize novel materials/structures with enhanced Spin Seebeck coefficient / figure of merit.

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 seven 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. Pani Varanasi, ARO, 919-549-4325,

Chakrapani.v.varanasi.civ@mail.mil; Dr. Mark Spector, ONR, 703-696-4449 mark.spector@navy.mil

ARO FY2013 MURI TOPIC #6

Submit white papers and proposal to Army Research Office

Transforming Information within Nonequilibrium Nanosystems

Background: Several experimental breakthroughs in the nanosciences have opened new possibilities for the creation of synthetic nanosystems capable of exploiting information for a broad range of novel functions. In particular, recent progress has shown that the thermodynamic cost of stored and released information, together with feedback control, can be utilized to efficiently direct molecular transport and even increase the free-energy of nanoscale fluctuating particles. These results build upon a steadily increasing understanding of the deep connection between information theory, nonequilibrium physics, stochastic dynamical systems, and feedback control at the nanoscale. While free-energy transduction or explicit utilization of directed molecular transport has yet to be demonstrated, several years of progress and interest concerning the development of artificial Brownian motors suggest the potential for an exciting future of autonomous nonequilibrium nanosystems capable of performing meaningful work with remarkable efficiency. Greater understanding of complex nonequilibrium interactions and information processing may lead to new directions concerning synthetic nanosystems capable of manipulating emergent phenomena. Information-based feedback control within nonequilibrium nanosystems has emerged as a promising and novel approach toward the next generation of synthetic nanosystems.

Theoretically, much recent progress has been enabled by several advances in nonequilibrium physics to include the Jarzynski and Crooks fluctuation theorems, the nonequilibrium temporal ordering theorem, and enhanced understanding of the emergence of statistical behaviors based on nonlinear dynamics. However, these foundations remain limited and have not fully developed the connection between nonlinear dynamics and intrinsic information flow within more general dynamical systems or how systems interactions and feedback influence nonequilibrium dynamics and information processing. Research results concerning nanoscale feedback control which, in turn, led to results generalizing the Jarzynski theorem and the first demonstration of a Szilard engine attests to the opportunity for further multi-disciplinary basic research. Experimentally, demonstrations have also been mostly relegated to single-particle systems with macroscopically implemented and non-robust feedback control. Next generation nanosystems will need to be not so constrained. Hence, this MURI will pioneer the fundamental principles underlying novel techniques for exploiting nonequilibrium dynamics, information, and feedback control to perform useful work and directed motion within nonequilibrium nanosystems.

Objective: The objective of this MURI is to develop fundamental understanding of the nonequilibrium thermodynamics of information processing and feedback-control within nonlinear systems at the nanoscale. Such understanding will enable synthetic nanosystems capable of robustly controlling changes in free-energy, entropy production, and momentum.

Research Concentration Areas: Suggested research areas include, but are not limited to the following: theoretical approaches (nanoscale statistical physics and information processing grounded in the first principles of nonlinear dynamics;); nonlinear and stochastic mathematics (fractal processes, stochastic versus deterministic modeling); mechanical and electrical engineering sciences (nonequilibrium work cycles; novel approaches for nanoscale sensing and actuation; control in the presence of Brownian motion); experimental approaches (new methods to accomplish nanoscale transport, directed motion, and information-to-energy conversion; artificial molecular motors).

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 six 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. Samuel C. Stanton, ARO, 919-549-4225, samuel.c.stanton2.civ@mail.mil

ARO FY2013 MURI TOPIC #7

Submit white papers and proposal to Army Research Office

Controlling Collective Phenomena in Complex Networks

Background: Descriptive understanding of the structure and function of complex networks, from genomic transcription to cooperative decision-making, has recently shown significant advancement. Thus far, descriptive modeling of emergent behavior in complex networks has shown a strong linkage between network dynamics and topology. Recently, two major hypothesis that provide insight to the connection have evolved; (1) define the system with a static complex network topology that drives nodal dynamics, or, (2) define the network structural topology itself as a dynamical system where the nodal dynamics play only a minor role. Both lines of research have separately improved our understanding of complex networks. The first provides insight into linkages between synchronization, topology, ensemble size, and aggregate behavior, while the second provides insight about the relationship of small-world and fractal scale-free networks, resilience and robustness. Future efforts that build on this understanding with an eve toward controlling the behavior of complex networks will require creation of a new mathematical infrastructure that dovetails these approaches. In particular, a new analytical framework is needed that considers more realistic networks that *co-evolve* and *adapt* with the dynamics of the underlying topology, and that formally characterizes the crucial feedback mechanisms linking both structure and dynamics. For complex general networks the role of hierarchical organization and multiscale phenomena present significant challenges, the absence of any physical intuition or formalism makes finding solutions particularly problematic. Fortunately, there has been significant progress over the last several years concerning the behavior of adaptive and coevolutionary networks [J. R. Soc. Interface 2008, 5, 259-271; Phys Rev Lett, 108, 114101 2008; Nature Sci Rep. 2011, 1:99 doi:10.1038/srep00099]. In addition, contemporaneous research on implementing nonlinear feedback has lead to new concepts for engineering the collective dynamics of nonlinear oscillator ensembles [Science, 316, 1886-1889; Science, 316, 1857-1858; Phil. Trans. R. Soc. A., 2010, 368, 2189-2204] and may also be applicable. Most recently, a controversial theory has been proposed that bridges fundamental principles of control theory with complex directed networks [Nature 2011, 473, 167-173]. To this end, a multidisciplinary effort is necessary to make substantive progress in this area, one that capitalizes on recent breakthroughs in network science and leverages progress in the nonlinear dynamics of Boolean networks, evolutionary game theory on networks, and switching networks.

Objective: The objective of this MURI is to develop the theoretical foundations for novel capabilities to control and exploit collective phenomena and diffusion within adaptive, co-evolutionary complex networks. A successful proposal will present generality of the results across a broad range of data sets and experimental test beds.

Research Concentration Areas: Potential research areas may include, but are not limited to, theoretical methods from control theory, statistical physics, nonlinear dynamics, microeconomics and game theory to understand adaptive, co-evolving networks across disparate disciplines and feedback architectures in natural systems. Experimental and simulation methods may be drawn from high-dimensional MEMS/NEMS oscillators, neuroscience, sociology, and condensed matter systems. The dynamics and control of ensembles of nonlinear oscillators, as both descriptive models and true physical entities, are likely to permeate both approaches.

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 six 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:

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ARO FY2013 MURI TOPIC #8

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Physiochemical Determinants of Cognition and Decision Making

Background: The neural pathway of the chemical sense passes directly to the amygdala and hippocampal formation of the limbic system. The primacy of the olfactory system in ontology and its direct connection to critical areas in the formation of emotional and autobiographic memory implicate olfaction as a primal sense governing behavior. Odors are reasonably considered as harbingers of disease, markers of physiological state, and modulators of memory and emotion. Malaria, "bad air", may be derived from the conditioned association between the stench of stagnant water and the disease. The association between a smell and illness is powerful, often conditioned in a single trial and resistant to extinction. This associative power with well being is often leveraged in alternative or complementary medicine practices of aromatherapy. Individuals tend to prefer certain odors, masking offensive scents and augmenting preferred ones. Arguably humans can differentiate individual odors based on kinship, as has been demonstrated in animal models. These odors may arise from shared familial or cultural diet, genome, hygienic practice or some combination. Historically, military regiments came from geographically confined areas with genomically similar individuals, who were kept together to maintain loyalty and cohesion. Hypothetically, some of the group identity was maintained via in-group shared chemical signals, which are now assayable in zeptomole (one sextillionth) quantities. There is evidence that trust and other affiliative behavior is governed by oxytocin and is reflected in functional brain imaging studies. Olfactory mechanisms are implicated in neural pathways. Several questions arise that are addressable by an iterative process between modeling and experiment: What are the olfactory mechanisms of trust; which metabolites influence identification within a social unit; can shared genomic profiles act as selection/exclusion criteria for affiliation; can shared experiences modulate group odorant signals; what are the modulating influences of commensal micro-organisms; can quantitative predictive models be constructed using sensory inputs including concentration levels, chemical composition, and temporal-spatial distribution that relate individual and group decision making or consensus building to both internal and external human physiochemistry?

Objective: Determine how odors are formed, maintained and modulated by genetics, sex, gender, diet, commensal microorganisms, and social structures to enable the use of personal and group odor in generating supra-individual identities.

Research Concentration Areas: Approaches may include, but are not limited to the following: 1) Genomic and metabolomic determinants of eccrine, sebaceous and apocrine gland secretion contributions to individual odor profiles, 2) Identity of the chemical compounds of individual and group odor profiles that depend on diet and on the activity of the biochemical pathways that generate these compounds, 3) Commensal microorganism population makeup and variability, within and between groups of socially bonded individuals, 4) Determinants and cognitive sequelae of rates of odor profile change as a function of exposure to group odors, 5) Quantification of psychosocial effects of odor variance within and between groups as a function of time, stress, physiological status and shared experience as well as effects on other senses, 6) New mathematical modeling techniques to support nonlinear, dynamic conditions inherent in neural behaviors involved in reacting to olfactory stimuli, 7) Characterization of cortical excitatory-inhibitory neuronal network mechanisms underlying spatiotemporal patterns in the biophysical data.

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 five 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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Measurement and Verification Methods in Quantum Information Science

Background: With the advent of a new generation of semiconductor technologies that make use of quantum states, often at room temperature, there is a need for algorithms that exploit these new capabilities. Such algorithms could exploit the new devices for transformational computational strategies, improving communications capacity, and securing information transactions. One area of quantum information science that must be improved is in the area of quantum measurement and verification. Thus with methods in error correction and quantum computation, or security protocols with quantum communication, estimation of the true state of the quantum system is needed in the context of system measurement noise and uncertainty. In parallel, logical methods in program verification, and model and equivalence checking, have been the norm in formal methods.

The immediate impact of this work would be a new class of protocols that would allow the estimation and detection of quantum states, for verification of the behavior of new semiconductors and network architectures. The broader impact of this work would be in many areas, from the physical and biological sciences, to computer, communications, and systems engineering, and information security. Thus if a low dimensional set of states could predict the outcome of a global system's behavior, new protocols could be designed for materials analysis, biological system identification, information assurance, and verification of the performance of heterogeneous systems. Application areas of interest could involve optical room temperature quantum semiconductor design, protocols for materials design and analysis of biological materials, network information assurance, and verification of large software and hardware infrastructures.

Objective: Our objective is to unify quantum measurement strategies with logical verification methods for a unified measurement-based quantum verification approach. Thus strategies that can perform local measurement of a quantum system and infer the global state space of the system are of interest. From these properties we hope to infer different categories of logical outcome such that if measurement is performed on local regions of a quantum system, we can determine whether a particular computational or communications system result was achieved. Additionally, these measurement strategies would need to be robust to noise and system performance characteristics such as poor sensor performance, temporal, phase, space, and frequency resolution issues, and scale less than exponentially with the number of qubits in local and distributed measurement settings .

Research Concentration: Suggested research areas include but are not limited to: (1) Methods in sparse approximation in the measurement of large systems, geometric information theory, Bayesian estimation, and algebraic statistics; (2) Statistical models of quantum systems such as weak coherent state and single photon quantum regimes. (3) Methods that derive from operator, quantum representation, random matrix, mean field, and renormalization group theory, as well as topological statistics (4) Methods in equivalence and model checking, domain theory, probabilistic process algebras, as well as sheaf, and category theoretic verification methods.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an average of \$2.5M per year for 5 years, supporting no more than 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.

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New Quantum Phases of Matter

Background: Cold atoms and molecules in optical lattices are ideal, precisely controllable model systems for exploring many-body phenomena, owing to the fact that the experimental systems are clean and understood ab initio, which allows for investigating condensed-matter physics in a more transparent and generic manner. The field of quantum simulation with cold quantum gases has been an active and fruitful area of research for the past decade, aimed largely at understanding the physical mechanisms behind the unusual properties of strongly-correlated materials, such as high-Tc superconductors, materials that present an intractable problem for conventional computational methods.

This MURI program aims to extend beyond condensed-matter systems that exist in Nature, to explore the wide range of possibilities for exotic quantum phases which might have extraordinary properties that in the future could be harnessed in a practical material. This exploration is enabled by dramatic recent developments of various novel experimental techniques for generating and probing exotic quantum matter. Cold-atom experimentalists today have control over many system properties including dimensionality, interaction, temperature, lattice geometry, orbital degrees of freedom, and quantum statistics (Bose vs. Fermi, and mixtures). In addition, they now have access to exotic quantum spin systems with SU(N) symmetries using alkaline-earth atoms, and have the ability to engineer artificial gauge fields and spin-orbit interaction. The latter has recently been demonstrated in atomic Bose-Einstein condensates, paying the way for experimental realizations of the theoretical paradigm of topologically-ordered quantum matter, such as quantum Hall states, that would, for example, provide full protection against errors in a quantum computer. Other important recent developments include quantum gas microscopy, novel lattice geometries, and ultracold dipolar matter. Quantum gas microscopy has opened the possibility to read out many-body quantum states in optical lattices at a single-atom level, enabling direct measurement of a variety of correlation functions. Novel lattice geometries have been realized recently, such as hexagonal, checkerboard, and Kagome lattices, as well as double-well superlattices. Such non-trivial lattices introduce a new low-energy orbital degree of freedom, opening the door to studying "orbital physics", i.e. the association of new types of long-range order, symmetry breaking, and non-equilibrium dynamics with the lattice geometry. Predicted phenomena include supersolid or quantum nemetic phases, the anomalous quantum Hall effect, and frustrated orbital magnetism. Recently achieved ultracold polar molecules and dipolar atoms introduce a new control parameter in the cold-atom tool arsenal - tunable long-range interaction, which allows for fundamentally new condensed-matter phases and new complex quantum dynamics.

Objective: The goals of this MURI include theoretical predictions, and experimental realizations with cold quantum gases, of exotic quantum phases of matter that do not exist in Nature. Such novel phases may include, but are not limited to: topologically-ordered quantum matter, novel superconductors, spin liquids, supersolids, quantum liquid crystals, and non-Fermi liquid metals. It is expected that as-yet unknown phases will be discovered as well.

Research Concentration Areas: This is a broad multidisciplinary effort where theory and experiments are envisioned to be closely connected. Research concentration areas should include production of novel states of matter, novel methods for probing and measuring the properties of such states, and theoretical prediction of as-yet unknown quantum phases.

Resource Allocation: It is anticipated that awards under this topic will be no more than an average of \$2.5M per year for 5 years, supporting no more than 8 funded faculty researchers. Exceptions warred by specific proposal approaches should be discussed with the topic chief during the white paper phase of the solicitation.

Research Topic Chief: Dr Tatjana Curcic, AFOSR, 703-696-6204, Tatjana.curcic@afosr.af.mil.

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Multiphysics and Multiscale Failure Prediction through Peridynamic Theory

Background: A traditional challenge in materials science is to control the complex non-linear relationships between mechanical properties and failure criteria. The current paradigm of *predictive materials modeling and design* requires extensive use of finite element analysis but traditional approaches for dissimilar materials (heterogeneous structures) do not accurately take into account of the governing physics in these dissimilar materials. Failure prediction is also not physics based because complex crack propagation paths and patterns are not known apriori. The stress and strain fields of these material systems are discontinuous – requiring special treatment for each case and external failure criteria for crack propagation. Multiscale material models that account for structure variability at different scales pose significant mathematical and computational challenges not addressed by such traditional multiscale approaches. These issues become even more important as many problems of interest are posed as materials design problems in the Materials Genome Initiative, one goal of which is the certifying of materials leading to predictable and desired performance at the macroscale.

The peridynamic model of solid mechanics replaces the partial differential equations of the standard theory with integral equations. These integral equations remain applicable to deformations containing discontinuities; thus they can be applied directly on an advancing crack tip. Unlike the standard theory, the peridynamic model also allows for direct force interaction between continuum particles separated by finite distances. Therefore, the peridynamic model is inherently nonlocal. Because the fundamental equations can be applied directly on a crack or other discontinuity, the peridynamic model does not use the special techniques of fracture mechanics, such as supplementary kinetic relations that dictate when a crack should advance. This suggests that the peridynamic approach may have the potential to treat multiple, mutually interacting cracks in more generality than the standard theory allows. It also suggests a natural

way to treat damage in heterogeneous media such as composites¹.

Objectives: The objective of this MURI is to establish mathematical approaches for the peridynamic theory in order to demonstrate and simulate cyclic combined loads and to develop a unified bond-based and state-based peridynamic theory capable of predicting the response associated with combined loads (e.g., thermal, mechanical, acoustic and others) for dissimilar material systems within a statistical framework for multiscale materials modeling. Researchers from material science and engineering along with applied mathematicians and statisticians are encouraged to develop Information theoretic approaches to provide predictive models for multiscale damage progression and successfully resolve issues of complexity, variability across time and length scales, and allow for a dynamic integration with new experimental methods of rapid validation of structure and properties at different scales.

Research Areas: Particular topics of importance to this MURI include but are not limited to 1) Development of new multiscale multiphysics peridynamic theory that can realistically capture crack initiation and formation. Approaches that can provide a generalized science platform for the quasistatic and transient analyses, thermal loading, material and geometric nonlinearity, dissimilar materials with distinct interface properties, presence of complex geometry and variational theory, conditioning, and domain decomposition for nonlocal problems 2) Demonstration of Peridynamic theory at different length scales (meso-, micro-, and nano-scales) for different external fields, and adaptive dynamic relaxation conditions of the structure under

external fields 3) Demonstration of capability to predict coupled field analysis; i.e., thermoelectromechanical loading (electromigration phenomenon – atomic diffusion, state of electrical-, thermal-, and mechanical fields); 4) applicability to simulate fabrication processing at the different length scales (sintering, void formation and material removal). The introduced

techniques need to be able to produce quantifiable property variability utilizing a determination of peridynamic material models from ab-Initio lattice dynamics calculations and multiscale dynamics of heterogeneous media in the peridynamic formulation.

In all of the research areas described above, validation of the newly developed theories and models by comparing to experiments is expected. Use of existing experimental data is acceptable provided that sufficient characterization of the experiments, i.e. all of the important characteristics of the experiment that are needed for the simulation, have been demonstrated. Supplemental experiments or new experimentation may be necessary to verify and validate the theoretical advances and computational simulations.

Resource Allocation: 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.

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Electrochemical Dynamics in Nanoscale Systems

Background: Electrochemistry is the branch of chemistry that explores the relationship between chemical processes and electricity. As such, it provides the theoretical and experimental tools to probe and directly couple to energetic electronic processes in functional materials systems such as: (i) portable electronics and electromechanical systems, where electrochemistry often provides the requisite potential driving forces (voltage) and electrons (current); (ii) biological systems, where electrochemistry is the basis for the energetics of living systems and is a versatile probe of ions and redox active molecules involved in biochemical processes; and (iii) photovoltaic and electroluminescent systems, where electrochemical redox couples can be designed to perform photon-to-electron interconversions for enerav harvesting and light generation technologies. With the continuing explosion in nanoscience and nanotechnologies, new breakthroughs are possible in many areas that require an understanding of electrochemical dynamics at the nanoscale, including: (i) nanoelectronics and nanoelectromechanical systems (NEMs) providing increased computational and information storage capabilities at exceptional low powers - memristors being one such recent breakthrough that utilizes solid state electrochemical dynamics to vary resistance as a function of charge at the nanoscale; (ii) inherently nanoscale biological systems will become further integrated with the physical sciences, requiring effective nanoscale linkages to interface biochemical processes with physical chemical responses - electrochemical dynamics can serve as this interfacial couple; (iii) and quantum control over photon-to-electron will increase the efficiencies, spectral response, and lifetimes of photovoltaic and electroluminescent devices - electrochemical dynamics being the basis of such processes. While electrochemical dynamics offers great opportunities, accurate electrochemical theory and ambient experimental methodologies have been limited, for the most part, to dimensions down to only the sub-micron (>100 nm) regime. For electrochemistry to function as an effective dynamic couple to nano-S&T systems, new theoretical descriptions, experimental tools, and design methodologies for functional device design and fabrication must be developed to study and utilize electrochemical dynamics occurring at nanoscale dimensions (1 – 100 nm).

Objective: Develop the electrochemical dynamic theories, experimental tools, and methodologies for device design that will enable the application of electrochemistry as a linkage or probe for nano-S&T functional materials systems.

Research Concentration Areas: Areas of interest include, but are not limited to, the following: (1) theoretical treatment of electrochemical processes (*e.g.*, electron transfer kinetics and ion transport) at nanoscale dimensions (1 - 100 nm); (2) electrochemical probes with nanometer scale dimensional resolution (*e.g.*, scanning electrochemical "nano"-scopes); (3) effective experimental methodologies to link electrochemical probes with electronic, NEMs, and biological structures; (4) multifunctional probes for simultaneously evaluating electrochemical and photon response in nanoscale systems (*e.g.*, nanometer resolution imaging of electrochemiluminescence); and (5) novel electroanalytical methods to monitor and control ionic and electronic activity in biological systems.

Resource Allocation: It is anticipated that awards under this topic will be no more than an average of \$2.5M per year for 5 years, supporting no more than 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.

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A New Paradigm in Sources and Physics of High-Power Ionospheric Modification

Background - The DOD has long been interested in the impact of space weather on space assets. With a variety of energetic drivers, from solar wind to various plasma instabilities, the ionosphere is a complex, and hostile environment in which to operate missions critical to US dominance of the modern battlefield. Furthermore, we interact with our spacecraft through electromagnetic (EM) signals propagating through the ionosphere. This charged plasma environment provides a veritable zoo of plasma waves and instabilities that may contaminate these important signals leading to degraded radar and communications transmissions and precision navigation and timing. These effects naturally extend beyond the military world to other commercially critical space-based programs, such as the Global Positioning System, which is affected by phase modulation, energy absorption, and parametric frequency conversion that transfers EM energy to incorrect frequency bands. The parametric instabilities that play critical roles in the coupling of energy to the ionosphere are not completely understood and additional unexplained processes lead to high energy electrons that provide transport of energy out of plasma structures. These effects include, but go beyond, the amplitude and phase modulation due to scatting of electromagnetic signals involved in scintillation to broader fundamental questions of frequency conversion, wave mixing, plasma heating/cooling, and energy transport that result from active nonlinear nature of the ionospheric plasma. The military and scientific community has provided sizable investment in the development of High Frequency (HF) ionospheric heaters that provide the means to perform controlled experiments to study these questions. These facilities have been constructed using legacy electromagnetic sources. While highly reliable, their low power has resulted in a requirement for large antenna arrays to achieve the needed power level to impact the ionosphere. Given the large number of active elements, complex controls are needed and this, combined with the sheer cost of multiple sources, phase shifters, and antennas, leads to installations at a few fixed location worldwide. The geomagnetic field at given location is thus fixed, and the sensitivity of the coupling to the ionosphere in the different magnetic configurations cannot be studied, and this has significantly limited the scope of this research investment. Recently established new concepts in metamaterials operated at high power in directed energy devices present the potential for high power, low frequency sources of unprecedented compact size suggesting the potential to replace the current large collection of sources with a single, mobile, and cheap high-power amplifier with the capability to revolutionize the science and operations of ionospheric modification. While the energy density of this new source is projected to be lower than has already been demonstrated by the HPM community, it is anticipated that the lower frequency source will require the exploration and validation of new concepts for sources using metamaterials and active nonlinear materials. This can only happen with close collaborations of the space weather and source communities and active leadership of the PI to ensure the required teaming.

Objective – The goal of this effort is to bring together physicists and engineers from the space science, ionospheric modification, plasma modeling, and high power microwave source communities to examine anew the question of coupling electromagnetic energy to the ionosphere. The winning proposal will outline a program to combine the efforts of these communities to: 1. Perform fundamental research to determine the most important properties

of an EM source (frequency, amplitude, phase, waveform, etc) to answer the critical physics questions for efficient coupling to the ionosphere, including determination of optimal locations and ranges of ionospheric conditions; 2. Define, and design modern, efficient, powerful, and adaptive/tunable EM sources for ionospheric modification, and provide hardware testing under laboratory conditions typical at University high power microwave facilities (vacuum loads and/or anechoic chamber); and 3. Develop the theoretical tools and framework to design a feasibility

experiment to demonstrate and test the results of the research for ionospheric modification. In particular, this effort seeks to enhance the ability to create, diagnose, and control large scale plasma structure and artificial auroras to illuminate important fundamental nonlinear interactions in the ionosphere. The desire is that the scientific effort is synchronized with the design and laboratory testing of coherent electromagnetic sources to provide the optimum platform to understand the physics of the ionosphere. This understanding will facilitate the development of next-generation scientific tools for the space weather and heater communities for communication, over-the-horizon radar, and radiation belt remediation. Promising device and operational concepts from this MURI will be further studied and demonstrated with other agencies, such as the Air Force Research Laboratory.

Research Concentration Area – This effort will be focused on enhancing our understanding of EM energy interactions with the ionosphere made possible by optimizing state-of-the-art high power electromagnetic sources for this purpose. The goal is to dramatically improve both our knowledge of the non-equilibrium plasma physics in the ionosphere and our capability to push the boundaries of the electromagnetic spectrum of high-energy density electromagnetic sources. The combined communities of source and space weather physicists, pulsed power engineers, electrical engineers, and applied mathematicians are needed for the scope of this effort.

Resource Allocation: 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.

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Magneto-electric Energy Conversion Materials: Terahertz Emission and Efficient Energy Conversion in Unbiased Dielectrics

Background: Optical magnetization has received growing attention in the last three years for relevance to emerging fields like spintronics, quantum information science, optomagnetic data storage, and transformation optics. In most aforementioned topics, the optical coupling of light to spins has been based on intrinsically weak spin-orbit coupling effects in magnetic media. Yet, it was effective enough to support applications. Recent experiments, however, confirmed that the Molecular Dipole (MD) radiation intensity can be as high as one quarter of the intensity of electric dipole (ED) radiation. The combined interactions of dynamic magnetic and electric fields can be parametrically enhanced by over eight orders of magnitude in transparent dielectrics, on an ultrafast timescale. This newly-discovered nonlinear optical phenomenon is called magneto-electric conversion (MEC).

A remarkable feature of this energy conversion is based on induced voltages between the surfaces of dielectric optical materials, forming an "optical capacitor". The process itself requires parametric down conversion driven by optical E and B fields, and this energy transfer produces static charge separation in atoms irradiated with intense light. The magneto-electric power generation phenomenon relies on displacement currents in insulators, and avoids both the absorption and electron-pair production that typify semiconducting solar cells. Magneto optic has long been considered the poor cousin of electro optics. Yet, Rasing, Kimel and Stavciue demonstrated that ferromagnetic domain flips with single 100-fs laser pulses showing a possible indication of giant spin-orbit coupling. Dynamic effects from the product EB have been overlooked because the combined force of E, B is not derived from an atomic potential (EB is not energy density). EB-driven dynamics arise from energy-transfer process, and combines both nonlinear and nonequilibrium phenomena. This signifies the fundamental objective of this basic research initiative, to uncover, explain, and exploit this new science of MEC materials. The conversion process produces no heat, utilizes low-cost, transparent dielectric materials and offers the prospect of nearly unit efficiency in the transformation of light energy into electricity. Its key advantages can be traced to the temporary evasion of thermal relaxation while inducing charge separation in the ground state of atoms or molecules. Surprisingly, coherence of the input light is also not required, so MEC should enable direct conversion of light into electricity whether the input is in the form of sunlight, laser beams, or other forms of directed energy. This offers new capabilities for power beaming to support air and space constellations of DOD assets.

Objective: The ultimate aim of this initiative is to establish the framework required to develop a new and revolutionary class of materials capable of sustained operation of magneto-electric conversion. The objectives of the proposed effort are: (1) to gain an improved understanding of the mechanism of new nonlinear optical effects, (2) to investigate their response to coherent and incoherent radiation, and (3) to guide a transformative scientific advances in optical energy conversion. The prerequisite is the understanding how the magnetic component of light can join forces with electric field to drive unanticipated optical response. These objectives require the systematic study of dielectric materials with centro-symmetric and non-centro-symmetric materials through first principles electronic-structure calculations

based on density functional theory to improve models, to elucidate the role of symmetry, and investigation of non-linear optical effects and their relation to thermodynamically stable material systems that can act lossless media for conversion. By performing baseline studies of magneto-electric rectification, this basic research initiative has the added objective to furnish design rules for novel energy conversion processes.

Research Concentration Areas: Analysis to date has explained some puzzling aspects of this new phenomenon, but the prominent role ascribed to the optical magnetic field involves unique dynamic enhancement that needs to be much better understood by the work of four research communities. Specific disciplines of 1. material science, 2. physics, and 3. applied mathematics are necessary to achieve this understanding. Further exploitation and understanding of this phenomenon suggests that additional researchers from the 4. electrical engineering will strengthen the team.

Resource Allocation: 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.

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Photonic Synthetic Matter

Background: The fundamental symmetries of parity and time are now being exploited to enable the spatial guiding and selection of propagating radiation, and could ultimately underpin a new generation of sophisticated, integrated photonic devices. Parity-Time (PT) Symmetric Materials is a class of theoretically conceived materials that does not exist in nature. Much like negative-index materials, it is based on an abstract set of mathematical properties governing electromagnetic wave propagation. It initially emerged within the context of quantum field theory as a novel theoretical construct. Mathematically speaking, a physical system exhibits Parity Time-symmetry provided that a physical trait of the system is invariant under the combined action of spatial and time reversal. In the past few years, the possibility of PT-symmetry was theoretically introduced and experimentally demonstrated (proof of principle) by several groups. One-dimensional PT-symmetric systems have been achieved by fabricating a material-system in which optical loss is judiciously balanced by optical gain via inversion symmetry. Suitably configured PT-symmetric materials will allow unusual control of how waves propagate through the materials. For example, PT concepts can provide new strategies to introduce gain in many optical metamaterials and plasmonics systems that have so far been plaqued by losses. Scattering from PT structures can be appropriately engineered to induce an abrupt switch to a new state of behavior which can provide opportunities for designing new laser structures and, alternatively, coherent perfect absorbers or anti-lasers. Polymer processing will allow the fabrication of 1D (waveguides), 2D (Bragg arrays), and 3D (nano- and micro-scatterers and whispering gallery resonators) structures, which would be difficult to achieve with other materials. The flexibility of polymers is a valuable asset that allows, for example, the fabrication of structures that may conform to non-planar geometries or configurations such as the external surface of an aircraft. During this effort, the potential of PT-symmetry will be explored by conducting further theoretical studies of these structures through modeling and simulation and extending the PT-symmetry concepts beyond the optical regime. Unusual wave propagation control will be explored by extending the 1D demonstration to fabrication of complex 2D and 3D structures through advanced polymer processing techniques.

Objective: To explore and to achieve 1D, 2D, and 3D PT-Symmetric structures in the optical regime and to extend the PT-Symmetry concept beyond the optical domain.

Research Concentration Areas: (1) Theoretical studies involving both modeling and simulation methods to analyze the optical behavior of PT-symmetric systems in higherdimensions and under vectorial or nonlinear conditions will be pursued. Exploration of the concepts and models beyond the optical regime to other quantum domains of open systems will also be undertaken. (2) Utilization of advanced self-assembly approaches such as engineered specific interactions, nano-domain phase separation control, and advanced multi-component fiber spinning processes to achieve multi-dimensional PT-symmetric systems. (3) Perform experiments to characterize these PT-symmetric systems and to validate theoretical predictions. Also explore how optical isolation can be enhanced with such materials in the context of photonic monolithic integration for next generation photonic monolithic circulates, like RF engineered semiconductor lasers.

Resource Allocation: 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.

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Random Lasers, Nano-spasers and Optical Rogue Waves

Background: The typical view of a laser is a gain medium in a cavity with mirrored ends. Recent discoveries have opened a new approach to laser realizations based on light undergoing complex multiple scattering in random media. It has been found that localized modes of light in random media can coherently enhance stimulated emission of radiation from atoms to produce laser light. These materials are called <u>RANDOM LASERS</u>. The laser light so produced can be simultaneously shining at several different frequencies. These frequencies can be tunable as temperature and pressure changes can produce changes in the material that alter allowed wave modes. A plethora of materials are candidates for random lasers including organic nanofibers, Cr doped ZnS nanocrystals, nanostructured thin films, semiconductor powders, cold atoms, ZnO/ZnMgO quantum wells, polymer films, metamaterials, photonic crystals and biological cells.

For visible light the minimal optical cavity size is about 150 nm (a half wavelength). Smaller laser sizes are possibly achieved through inclusion of metallic nano-particles to support localized surface plasmons. In this Surface Plasmon laser, the <u>SPASER</u>, plasmons are coupled to photon modes creating a nano-scale laser. The study of these random lasers potentially offers an easy to fabricate, miniaturized, inexpensive device able simultaneously to produce a spectral array of laser frequencies.

A fascinating nonlinear dynamic phenomenon, <u>OPTICAL ROGUE WAVES</u>, has recently been discovered in photonic crystal fiber lasers and in the propagation of light in a VCSEL semiconductor laser. Super-continuum light generation in optical fibers was found to produce large amplitude optical solitons that, in analogy to large ocean waves that can appear even in calm seas, have been called "optical rogue waves". A soliton wave is a super stable wave structure that balances nonlinearity with dispersion and is capable of long distance transmission without any spreading of the wavepacket. In the VCSEL, apparently noise can be amplified by positive Lyapunov exponent (chaotic) nonlinear processes to create a high intensity optical soliton. The parameter space of frequency vs. pump current shows a fractal set of regions where rogue waves can be produced. In another area, an unexplained phenomenon of hot-spot freak waves have similarly been observed in microwaves scattering from disordered metallic arrays.

Objectives: (i) Experimentally and theoretically explore the phenomena of wave generation, propagation, and scattering in a complex disordered medium especially_random laser and spaser responses. Electric and magnetic control of plasmons in spacers has yet to be explored but offers the promise of new sensors, switches, and magneto-optical devices. (ii) Study the generation and propagation of optical solitons in photonic crystals and semiconductor materials leading to the creation of optical rogue waves, (iii) explore random scattering freak hot-spot microwaves.

Research Concentration Areas: The research areas include but are not limited to (i) random lasers and spasers, (ii) nanomaterials, (iii) photonic crystals (iv) optical rogue waves (iv) microwave scattering freak hot-spots.

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 7 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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Free Space Optical Quantum Key Distribution (QKD)

Background: Quantum Information Sciences have become a rapidly developing field with considerable research effort expended in the development of quantum bits (QBIT) and strategies to support quantum computation (QC). In parallel with efforts devoted to computation, it has long been recognized that the mathematical framework associated with quantum mechanics would enable secure communications without the need for additional cryptographic systems. Bennett and Brassard (BB84) proposed a method for secure communications based upon the use of non-orthogonal bases in 1984 that has been experimentally demonstrated in a number of settings. Since the publication of the BB84 protocol additional protocols, such as the Ekert 91 protocol (E91), have been proposed that exploit quantum entanglement to insure secure communications. Regardless of the protocol, practical implementations of the protocol introduce errors arising from the inability to precisely implement the underlying mathematical structure that is being exploited in physical hardware. Since it is currently impossible to distinguish between the effects of these errors, and the presence of an eavesdropper within the QCs channel additional tools such as privacy amplification and information reconciliation have been developed and implemented.

Much of the research effort devoted to QCs has involved the use of nod-dispersive fiber optics with low loss. However, there are a number of circumstances in which communications over a point-to-point optical link are desirable. To date experimental demonstrations of QC protocols have occurred in relatively benign atmospheric conditions, such as between mountaintops, or mountaintops and satellites. These experiments have also demonstrated relatively low effective bit rates in comparison to fiber optic implementations. Of interest to the this MURI is developing a fundamental understanding of issues that currently prevent physical implementations of high effective bandwidth, long range provably secure QCs in challenging environments. These environments are characterized by dispersive, time varying atmospheres with significant scattering, and transmitters and receivers that are in motion. This leads to a desire to understand the fundamental issues associated with the efficient generation, propagation, entanglement, and detection of high repetition rate single photons.

Objective: The objective of this MURI is to develop an understanding and advance the capability for generating, propagating, entangling, and detecting photons, as well as creating new capabilities to maximize the information that a single photon can carry in free space. A multidisciplinary research effort will bring together mathematicians, physicists, computer scientists, electrical engineers, and astronomers together to achieve the objective of this MURI.

Research Concentration Areas: Suggested research areas include but are not limited to: (1) developing and understanding high repetition rate generation of entangled photons, (2) studies leading to an understanding of how to manage the propagation of photons in challenging atmospheric conditions, (3) development and understanding of novel mechanisms for single photon detection that support high frequency operation (4) development and understanding of schemes for hyper-entanglement of photons to increase the information carried by a single photon.

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.

Research Topic Chief: Dr. Carey Schwartz, ONR, 703-696-7824, carey.schwartz@navy.mil

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Integrated Nanophotonics

Background: Modern optical switching and modulation technologies have had incredible success coupling rapid scientific advances into innovative designs that support what is popularly known as the information superhighway. While these optoelectronic devices enable the high volume transport of information through both commercial and defense networks, they continue to be speed, size, loss and efficiency limited. Future demands for broadband signal transmission and processing will require optical switching and modulation rates that will support ultrafast (<1 psec) and extremely low energy optical switching/modulation not possible with current approaches. In addition, very large arrays of more moderate speed, but extremely compact, low insertion loss, and energy efficient switching fabric are needed to support the current trend of computing technology, which have evolved into ensembles of computers in large data centers, where scalability, energy/bit, and systems complexity are of great concern. These networking requirements impact at multiple scaling levels including intra-chip, chip-tochip, board-to-board, point-to-point and beyond. While digital signal transmission is critical, the potential for analog signal processing and transmission is equally compelling with orders of magnitude greater bandwidth available than that supported by electronic approaches. This MURI aims to explore new opportunities in emerging nanomaterials and nanofabrication technologies to overcome fundamental linear and nonlinear photonic switching and modulation limits across the extreme GHz to THz frontier.

Recent advances in understanding near field interactions of optical fields with artificially created inhomogeneous composite materials (e.g. metamaterials dielectrics, semiconductors, semimetals, metals, organics, and quantum dots) have established the opportunity for synthesis of new classes of material that will enable new families of linear and nonlinear nanophotonic devices. The nanometer scale geometries and initimate integration of these photonic devices will require investigation of methods to both mitigate and leverage guantum mechanical effects. Early investigation of sub-wavelength scale lasers, modulators, amplifiers and filters have yielded extremely promising results and provide confidence that this research will be scientifically fruitful from both a classical and quantum mechanical perspective. Ultra-low threshold lasers and extremely high quality factor optical cavities/resonators are a few examples of where nanophotonics has led to unprecedented performance advancements and reduced footprints compared with conventional large geometry device approaches. Current photonic activities exploring metallic plasmonic behavior and devices, and laser development efforts focused on coupling quantum dots with metamaterial structures provide further evidence that sub-wavelength linear and non-linear optical switching and modulation phenomena can result in fundamentally new science and engineering. The pursuit of the microscopic to macroscopic connection of nonlinear optical phenomena, new fundamental basic physics, novel materials science, and sub-wavelength scale device engineering promises to deliver fundamental advances in the scientific understanding of electromagnetic interactions in materials at the nanoscale. Concurrent advancement of the speed, size, loss and efficiency of nanophotonic switching/modulation phenomena towards fundamental limits will dramatically expand the ability to control and process large volumes of information.

Objective: The objective is to develop novel nonlinear artificially engineered material structures for low loss, high efficiency switching/modulation devices and arrays exploiting near field electromagnetic interactions coupled with quantum phenomena. These new materials should

use dielectric, semiconductor, semi-metal and metal compositions with topologies to enhance second and third order nonlinear optical coefficients avoiding slow responses close to resonance. The project is focused on pushing the limits of high-speed sub-wavelength photonic switching device structures and integration with minimal associated losses, and not focused on electronics integration or quantum information processing related technology. The research will pioneer a clear path towards improving fundamental switching efficiency limits in photonic materials and structures in the shrinking geometries enabled by emerging nanomaterial and nanofabrication techniques.

Research Concentration Areas: Areas of interest include, but are not limited to the following: (1) Experimental and theoretical study of the physics of near field optical interactions in nanostructured composite nonlinear materials, resonant nonlinear devices and integrated switching fabric; (2) innovative resonant materials and high-speed device structures for low loss optical and electrical switching, phase matching, and control; (3) develop modeling, simulation and optimization tools for investigation of nonlinear composite materials and switching/modulation devices; (4) nanofabrication of nonlinear nanocomposites compatible with processing of THz electronics; (5) nanophotonic characterization of amplitude and phase and near field interference effects.

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 7 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:

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Exploitation of Natural and Anthropogenic Noise for Ocean Exploration

Background: The conductive nature of seawater all but eliminates the possibility of probing the interior of the ocean by electromagnetic means. Optics can be quite useful at ranges from 10s to 100s of meters (depending on the water clarity), but at longer ranges acoustic methods stand alone as a means by which properties of the ocean can be sensed remotely. The ocean serves as an efficient channel for acoustic energy over a wide span of frequencies, and this information capacity has been leveraged since the first echo fathometers were developed in the 1920s. Recent decades have seen the development of many environmental sensing strategies that rely on relatively loud, controlled, and well understood sound sources that serve to constrain by suppression the information available for analysis. These constraints simplify the analyses and distill problems down to tractable numbers of input and output parameters, but exploration is limited to actively "illuminated" areas.

Ambient noise presents a useful alternative to well understood sound sources; it is analogous to ambient light, but much more challenging to work with. The amount of information that is contained within ambient noise (signals and channel characteristics) is often significant but not readily apparent and when viewed from a limited number of perspectives, appears to be hopelessly overlapped, but just as the listener attending a large reception can use selective attention to parse the incoming cacophony of acoustic information into perceptual "streams" of specific conversations, there are a variety of linear space, time, and frequency processing techniques that have been utilized to explore and extract information from ocean ambient noise. Bayesian approaches also hold a great deal of promise. When the streams are relatively loud or their features are known a-priori, any number of these approaches may prove useful, but exploration is often driven by experience and experimentation, as there is no systematic method or mathematical framework for determining the existence and quantity of meaningful information contained within an arbitrary large or high-dimensional ambient noise dataset.

Objective: The goal of this MURI is to develop the mathematical framework for determining the existence and quantity of meaningful information contained within large natural and anthropogenic noise datasets and improve methods for exploiting the information in support of environmental acoustic sensing.

Research Concentration Areas: The research of this initiative will concentrate on: 1) understanding the nature, utility, and variability of natural and anthropogenic noise sources in the context of environmental sensing, 2) developing the mathematical framework for determining the existence and quantity of meaningful information contained within large multidimensional datasets of ambient ocean noise 3) improving linear and non-linear methods for exploiting the information in support of environmental acoustic sensing.

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 7 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. Robert Headrick, Ocean Battlespace Sensing Department, Office of Naval Research, <u>bob.headrick@navy.mil</u>, tel. 703 696-4135

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Replacing Strategic Elements in DoD Materials

Background: The angst surrounding scarce and strategic materials availability has prompted numerous workshops and policy studies focusing on mitigation. Potential actions in the US, EU and Japan include securing local and overseas resources, stockpiling, introducing recycling strategies and, developing alternative materials. In the past, replacement strategies relied on locating known, well-characterized materials and then engineering solutions around them. Such replacement approaches, however, are fraught with technological problems that often preclude success. A materials-mimetic solution to the current and future materials replacement problems is needed.

Objectives: The purpose of this research topic is to: (1) provide a theory-based scientific framework allowing one to replace *any* element in a material such that the substitute material retains the original characteristic performance. This might be as simple as an isosteric substitution strategy, or one more complex that also includes multiple substitutions, either proximal or distal to the replacement atom and (2) verify and validate the strategy on a DoD-relevant material with the goal of being able to apply the approach to a broad range of materials. This project is not aimed at metallurgical alloy development per se, but instead is intended to explore new ways to mimic a given material (i.e., a material mimetic).

Research Concentration Areas: We seek new theories, new algorithms, and new computational protocols leading to rules and guidelines that will enable experimentalists to replace rare, expensive, or elements of strategic significance in a given material while retaining the core functionality of that material. Fundamental in this project is the discovery of how one might use substituting atoms alone, or in concert with (a) point defects like vacancies, interstitials, Frenkel, and antisite defects, (b) line and planar defects, and/or (c) bulk defects like voids to affect the requisite local charge density topology and thermodynamics. The research team may choose as a focus for the research activities any material, or critical element within an alloy or compound, of strategic interest. They are also free to consider either structural or functional (including catalysis) properties and performance targets. In their theoretical investigations, the investigators may pursue any approach of their choosing, including but not limited to: new quantum methods for ultra-high throughput screening of real or virtual compounds; mathematical extensions of cluster expansion theory or other techniques for predicting thermodynamically stable materials; informatics approaches and so on. In parallel with the theoretical investigations, however, the investigators must perform materials characterization and extensive experimental verification and validation of their theoretical approach. At the local scale, this should include characterization of local atomic and electronic structure and properties using techniques such as transmission electron microscopy, scanning probe microscopy, and local scattering spectroscopic techniques. They must also characterize the meso- and macro-scale properties requisite in the target applications of the materials system of focus in the project. At the conclusion of the successful project, the research team must provide: a set of general rules, guidelines, or strategies (that are transferrable to other classes of materials); and an appropriate proof-of-principle in which they predict a replacement material composed of non-intuitive and non-obvious atoms/atom placements and, subsequently, synthesize and evaluate that material.

Anticipated Resources: It is anticipated that awards under this topic will be no more than an

average of \$1.75M per year for 5 years, supporting no more than6 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:

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Acoustic Metamaterials

Background: The field of metamaterials has been rapidly developing, promising to deliver new materials with exotic properties such as negative refraction. Research over the past decade has led to a wide range of structures capable of controlling electromagnetic wave propagation over a wide spectrum from microwave to visible. These phenomena are a general feature of wave propagation, not confined to the electromagnetic spectrum. Recent research on elastic and acoustic metamaterials has led to several important theoretical advances that have introduced transformational acoustics, inertial metamaterials, and pentamode metamaterials. Initially acoustic metamaterials achieved negative effective bulk modulus and mass density through the exploitation of resonance behavior of the subwavelength constituent elements. Negative mass density has been achieved though the local resonances of individual mechanical constituents. Combining Helmholtz resonators to achieve negative effective bulk moduli one can design more complicated structures that have been shown to exhibit both positive and negative effective acoustic material properties. However, the application of transformation acoustics to these materials often requires extreme values in the material's effective mechanical/acoustic properties. Multiple scattering in crystalline or quasi-crystalline metamaterials can also be exploited to give a substantial range of effective physical properties in the homogenization limit. However, to achieve truly revolutionary metamaterials new concepts and subwavelength material components will be needed.

A unique feature of acoustic or elasto-acoustic materials is that they must be in physical contact with a background wave propagation medium, typically a fluid (water or air). This leads to significant hurdles since self-supporting solids have non-negligible shear moduli, whereas fluids manifestly do not support shear in the acoustic limit. Longitudinal fluid born waves can couple into both the longitudinal and shear modes of the solid causing serious deleterious effects upon acoustic response of the metamaterial. While the elastic wave equation does not have the required invariance properties to allow for the general use of transformation acoustics techniques, methods still exist to create metamaterials from elastic media for restricted cases. A recently developed class of elastic metamaterials, known as bimodal (2D) or pentamode (3D) materials, can be designed to support only one mode of wave propagation with an extremely low shear component, yet with a bulk modulus nearly that of a fluid. These materials could, in principle, ameliorate issues involving deleterious mode conversion in fluid-solid acoustic interactions.

Objective: The objective of this MURI is to discover new materials and structures that can be incorporated into acoustic metamaterials to achieve subwavelength spatial control of sound in three dimensions at audible frequencies. A multidisciplinary research effort will bring physics, materials science, mechanical engineering, mathematics, and electrical engineering together to design and synthesize these new constituent materials for three-dimensional acoustic metamaterials.

Research Concentration Areas: Suggested research areas include but are not limited to: (1) Theoretical tools (analytic and simulation) to design and characterize acoustic metamaterials, with particular emphases on understanding bandwidth and loss; (2) Fabrication techniques to build uniform structures with subwavelength composite features; (3) Demonstration of active acoustic metamaterials, which may be tunable, have gain, or show broadband properties; (4)

Exploration of acoustic devices to better understand the properties, benefits and fundamental limits of acoustic metamaterials.

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 7 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:

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Cognitive neuroscience of memory consolidation across sleep stages and efficient learning

Background: Recent results on the role of coherent brain oscillations in dynamically coordinating different brain regions have created strong interest in neuroscience. Evidence is emerging that the phase dependent spiking of neurons in relation to the oscillations in field potentials can code for objects in vision and short-term memory and support attention. One of the more remarkable observations to emerge from these studies is that sequences of actions or locations learned in waking are precisely, yet rapidly replayed in the hippocampus during high frequency ripple waves seen in slow wave sleep. These results are convergent with the strong emerging evidence linking memory consolidation and learning efficiency with sleep states. Interfering with slow wave sleep, or the transient high frequency bursts seen in hippocampus, produce deficits in episodic memory. Conversely, enhancing slow wave sleep, by transcranial stimulation of cortex or sleep sensory cues, enhances learning for declarative memory tasks. The incidence of these transient bursts is predictive of human test performance the following day. Evidence is emerging that tight coordination between hippocampus and neocortex during slow wave sleep promotes the consolidation of labile memories into stable memories for declarative, episodic learning. Moreover, the linkage between hippocampal ripples and cortical spindle waves occurs during transitions between cortical neuronal bistable "up" and "down" states. Across the sleep cycle, there is a specific sequence of sleep stages (slow wave sleep, REM sleep) that appears to be important for transforming the events and training of the prior day into stable memories and abstracted lessons. These exciting developments provide an opportunity to elucidate how specific neuronal population states and discharge patterns enable the connectivity, cellular and subcellular events of memory consolidation.

Objective: Conduct experimental and modeling research to elucidate how the biophysics of coherent brain oscillations and synchronized neural communication enable the consolidation of declarative memory for recent learning. Develop comprehensive accounts of how the neural events in sequential sleep states produce memory stabilization and abstraction at the levels of neuronal populations, neurons and synapses. Explore interventions that promote sleep events and sleep stages essential for memory consolidation and validate enhanced efficiency of learning in animals and humans.

Research Concentration Areas: a) Research that elucidates how the neural events across the sequence of sleep stages promote consolidation of memory for both declarative and procedural learning. b) Research on rational interventions to promote brain activity and sleep stages that enhance memory consolidation and learning performance that would be suitable for humans. c) Computational neuroscience and biophysical nonlinear dynamics modeling of the interaction among oscillating field potentials, neural activity, synaptic connectivity and cellular and subcellular processes involved in memory consolidation during specific sleep states.

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.

Topic Chief: Dr. Thomas McKenna, ONR341, 703-696-4503, <u>tom.mckenna@navy.mil</u> Participants: CDR Sheri Parker 342, Mike Shlesinger, ONR 30, Harold Hawkins, ONR 341, Ray Perez, ONR 341

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Computational Foundations of Moral Cognition

Background: Moral judgments are ubiquitous in our social interactions and are made anytime we make decisions concerning the welfare of others. Often, these decisions can have farreaching and serious consequences when applied in medical decision-making, politics, the law, and especially warfare. A collection of new studies by cognitive scientists is converging on a complicated picture of moral cognition as served by abstract reasoning within a folkpsychological network of concepts, affective responses to morally-tinged stimuli and as dependent upon other cognitive functionality including the ability to foresee the potential consequences of performing a moral or immoral action. In a complimentary line of work, a number of investigators are focused on elucidating the folk concepts we use in making moral decisions, including the nature of our mental representations of the self, other agents, freedom and responsibility. An initial systematization of these results will make them amenable to implementation within a computational cognitive architecture. Cognitive architectures are computational theories of the mental representations and processes that comprise human cognition. Recent work in cognitive architectures has focused on representation and reasoning about space, time, categories, action, uncertainty, and mental states such as beliefs, desires, and intentions. All of the aforementioned concepts play critical roles in moral cognition, and many of which seem to be the preferred subject matter for empirical study amongst cognitive scientists and others who are interested in moral cognition and its computational expressions.

Objective: To perform research and to develop enhancements to cognitive architectures supporting commonsense moral cognition and corresponding explanation, especially when prescriptive norms (e.g. the rules of warfare) don't adequately determine a unique course of action. Demonstration of research results in the form of proof-of-concept will be required. Relevant themes for demonstration might include planning in environments where the existence of wounded or injured teammates is a salient factor. Instances of this theme are many, but might include human-robot interaction during shipboard damage control or supporting casualty evacuation from the front line.

Research Concentration Areas: Topics might include but aren't limited to: the cognitive/neural architecture supporting moral cognition, the influence of emotions and motivations on moral judgments, the role of mental-state attribution in moral decision-making, representation and reasoning over moral content, and explanations referencing normative/moral content. Finally, an area of intense interest involves whether or not human users are better able to trust systems that (1) reproduce some of the variance seen in human moral judgment and (2) provide commonsense explanations over systems that implement a strict utilitarian calculus or a similarly strict set of permissions, obligations and forbiddances. Multidisciplinary contributions from psychologists, computer scientists, cognitive scientists, philosophers, neuroscientists and others are highly encouraged.

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.

Research Topic Chief: Dr. Paul Bello, ONR, 703-696-4318, paul.bello@navy.mil