

Contact Person	Duane Johnson [CRO]	Revision	4.0
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LDRD FY 2016 RESOURCES REQUEST PLAN

1.0 APPROVAL RECORD

- Reviewed by: Document Control Coordinator (Molly Daubs)
- Approved by: Chief Operations Officer (Mark Murphy)
- Approved by: Associate Laboratory Director for Sponsored Research (Deb Covey)
- Approved by: Assistant Director for Scientific Planning (Cynthia Jenks)
- Approved by: Chief Research Officer (Duane Johnson)
- Approved by: Deputy Director (Tom Lograsso)
- Approved by: Director (Adam Schwartz)

The official approval record for this document is maintained in the Training & Records Management Office, 151 TASF.

2.0 REVISION/REVIEW INFORMATION

The revision description for this document is available from and maintained by the author.

3.0 PURPOSE AND SCOPE

This document acts as official request for Ames Laboratory's annual LDRD expenditures.

3.1. Definitions

- LDRD – Laboratory Directed Research and Development
- LDRD Key Components:
 - *Strategic Initiatives* – employee-initiated proposals that address at least one of the strategic goals or an area of potential growth within AMES' initiatives for the current fiscal year.
 - *Novel Projects* – a balance of basic, applied, single-investigator, and multidisciplinary projects in new areas or directions, not necessarily in direct support of our strategic initiatives.
 - *Exceptional Opportunities* – an integral part of the pursuit of capabilities in a strategic area that enhances human and physical resources to support that area. This component consist of projects that do not fit neatly into the other two components or that can arise outside the normal fiscal-year schedule, e.g., strategic hires, collaborations with external institutions where a superior expertise resides, or projects offering exceptional R&D opportunities for AMES.

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4.0 PROGRAM/POLICY/PROCEDURE INFORMATION

In FY2016, Ames Laboratory requests approval for an LDRD expenditure comprising 3% of AMES' projected FY total costs, estimated to be approximately \$1.3M. The Director proposes a funding portfolio shown in **Tables 1 and 2** for the most current and next fiscal year, supporting the *Strategic Initiatives, Novel Projects, and Exceptional Opportunities*. These projects' datasheets are provided in addition to this Plan for DOE review and approval.

The Laboratory's request reflects management's best judgment as to the optimal balance between LDRD funds with their inherent flexibility and funds needed to accomplish programmatic deliverables for current sponsors while satisfying competing demands on Laboratory overhead. By insuring an adequate LDRD resource, laboratory management has a more effective tool to open new opportunities for creative Science & Technology directions and to adjust rapidly to new mission needs of the Department.

Due to the nature of exploratory research we cannot predict precisely to what program a given project may turn out to be most valuable over time. Nonetheless, the Congress of United States understands this role of exploratory R&D that underlies its granting the directors of national laboratories the opportunity to pursue laboratory-directed R&D and enables the laboratories to manage this vital resource and insure its productivity and relevance to the needs of the Nation.

5.0 LDRD Reporting

Annual LDRD program plan (this resource request plan) is required at Ames' Site Office at least 45 days before the start of the fiscal year. LDRD Portfolio Tables will be provided in 5.1.

In addition, a *summary report* from each principal investigator must be prepared for a brief annual report on their project within sixty days of the end of the fiscal year. An Office WORD Document Template prepared by LDRD Program is available from program office and website. The LDRD Program Coordinator compiles these individual reports and prepares an Annual Report on the LDRD program for submission, which is required within 6 months after the end of the fiscal year. The CRO, LDRD Program Administrator, and Budget will work together on Budget and Reporting to Site Office and DOE.

As required in Reporting Requirements (Section 7, [LDRD Plan 30000.001](#)), a "datasheet" template is required from each principal investigator during the approval process, so as to provide project summary information (Title, Brief Abstract, Lead Investigators, and Estimated Cost). Summary information from these datasheets goes to the Ames' Site Office, which will make them available to appropriate entities, including Congress. Datasheets must be submitted to Site Office at least 30 days prior to the start of the fiscal year to allow at least 30 days for review; for late-start projects, datasheets may be submitted any time in the fiscal year.

5.1. LDRD Portfolio Tables

The Director proposes a funding portfolio shown in **Tables 1 and 2** for the current and next fiscal year.

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TABLE 1.A FY 2015 INVESTMENTS (Actual)

	Distribution of LDRD Investment (\$K)	Planned Distribution of Investment (\$K)
Novel Projects		
FY13-15: Dynamic Whitelist Generation for Automated Intrusion Response	\$169	
FY15-16: Improving Ductility of High-Silicon Electric Steel (mid-year start)	\$37	
Novel Projects Subtotal	\$206	\$250
Exceptional Opportunities (<i>includes Spedding Fellows</i>)		
FY15-17: Studies of Novel Materials Using DNP-NMR Spectroscopy (<i>Spedding Fellow</i>)	\$138	
Exceptional Opportunity Subtotal	\$138	\$200
Strategic Initiative Areas		\$740
Materials Discovery and Design (MaDD) Science	Total: \$124	\$290
FY14-15: Self-healing, adaptive structural coatings <i>*project closed midyear</i>	\$17* (Approved \$70)	
FY14-15: Adsorption-induced, shape-change in nanoalloys: extended Wulff construction with first-principles calculations	\$57	
FY15-16 (late start): Novel modular thermal conductivity measurement setup	\$27	
FY15-16 (late start): Frequency-domain magnetic susceptibility under pressure and ultra-low temperature	\$23	
Greener Advances in Catalysis and Energy (GrACE)	Total: \$118	\$150
FY14-15: Customized Assembly of Catalytic Systems by 3D Printing Technology	\$118	
SS-NMR: Primary Research Initiative on Magnetic Resonance of Solid-state for Energy (PRIMROSE).	Total: \$297	\$300
FY14-16: Sensitizers for DNP-NMR Spectroscopy	\$175	
FY 14-15: Theory and Simulation of Solid-State NMR for Characterization of New Materials	\$122	
Strategic Initiative Subtotal	\$539	\$740
Subtotal	\$883	\$1,190
LDRD Administration Cost (estimated to EOY)	\$106	\$110
Total FY LDRD Funds	\$989	\$1,300 (approved)

TABLE 1.B FY 2016 INVESTMENTS (continuations included)

	Distribution of LDRD Investment (\$K)	Planned Distribution of Investment (\$K)
Novel Projects		
FY15-16: Improving Ductility of High-Silicon Electric Steel	\$50	
Novel Projects Subtotal	\$50	\$50
Exceptional Opportunities (<i>includes Spedding Fellows</i>)		
FY15-17: Studies of Novel Materials Using DNP-NMR Spectroscopy (<i>Spedding Fellow</i>)	\$183	
Exceptional Opportunity Subtotal	\$183	\$200
Strategic Initiative Areas		
Materials at the Edge of Stability (EdgeS)	Total: \$600	\$600
FY15-16: Novel modular thermal conductivity measurement setup	\$145	
FY15-16: Frequency-domain magnetic susceptibility under pressure and ultra-low temperature	\$93	
FY16: Development of high-pressure cell for magnetization measurements	\$96	
FY16: In-situ, real-time characterization of mechanochemistry processes by neutron diffraction	\$112	
FY16: TBA	\$154	
Greener Advances in Catalysis and Energy (GrACE)		\$160
FY16: TBA	\$160	
SS-NMR Sciences (PRIMROSE)		\$180
FY14-16: Sensitizers for DNP-NMR Spectroscopy	\$180	
Strategic Initiative Subtotal	\$940	\$940
Subtotal	\$1,173 (est.)	\$1,190
LDRD Administration Cost (estimated to EOY)	\$110 (est.)	\$110
Total FY LDRD Funds	\$1,283	\$1,300 (approved)

TABLE 2. LDRD PORTFOLIO INVESTMENT
(FY2016 are projected on approved LDRD funding level)

LDRD COMPONENTS	FY2014 (%) Actual	FY2015 (%) Actual	FY2016 (%) Projected	FY2017 (%) Projected
Novel Projects	23%	16%	4%	10%
Exceptional Opportunities [Projects] and <i>Spedding PD Fellowships</i>	0%	11%	15%	20%
Investments in Strategic Initiatives	60.5%	42%	73%	60%
FY 16-18: Materials at the Edge of Stability (Edges)	n/a	n/a	46%	35%
FY 13-15: Materials Discovery, Design, Development (MaDDD) Science	25.4%	10%	n/a	n/a
Greener Advances in Catalysis and Energy (GrACE)	21.0%	9%	13%	15%
Primary Research Initiative on Magnetic Resonance of Solid-state for Energy (PRIMROSE).	14.1%	23%	14%	10%
LDRD Administrative Cost	8.7%	10%	8%	8%
USED % LDRD	92.3%	79%*	100%	100%
UNUSED % LDRD	6.7%	17%*	0%	0%

* LDRD 3% rate was approved at estimated \$1.3M, but expenditures produced actual LDRD funds closer to \$1.1M (as of July 2015), which is 85% of approved amount. So, we utilized most of the funds generated under LDRD.

ADDITIONAL INFORMATION

FY2016 Strategic Initiative Area and Summaries

Materials at the Edge of Stability: (EdgeS)..... A-1
 Greener Advances in Catalysis and Energy (GrACE).....A-2
 Primary Research Initiative on Magnetic Resonance of Solid-state for Energy (PRIMROSE). A-3

A-1: Materials at the Edge of Stability (EdgeS): Manipulating Phase Transformation Functionality*

* This initiative replaces FY13-15: Materials Discovery, Design, and Development Science

Materials that respond vigorously to multiple external fields through phase transformations are responsible for many energy-conversion applications. **The Challenge** – Understand then predict the coupling of intrinsic and extrinsic effects to tailor the thermodynamics, kinetics, and microstructure to control reversible transformations and design responsive materials over a range of stress, temperature, and applied fields. As such, we will continue to expand a broader set of integrated capabilities for effective and efficient search methodologies for new energy-critical materials, including structure and chemistry prediction, with new functionalities. The new ideas and techniques will be coordinated with large-scale, predictive computational methods and new synthesis, processing and characterization to yield novel, valid design materials.

This LDRD thrust brings to bear synthesis and processing, advanced simulation, modeling and theory, as well as advanced in situ probes and characterization techniques.

The Goal – To enhance existing methods or to develop novel theory and experiment approaches to inform the synthesis and processing needed for new energy-critical materials with new functionalities, or characterization of unique materials.

Focus Areas for Potential Funding (not exhaustive)

1. Integrated computational rapid feedback for materials synthesis and processing of materials.
2. Optimization or algorithm development, e.g., for structural transformation pathways under application of various fields, ground-state prediction; structure-property data discovery
3. Synthesis and Processing, including new synthesis optimization protocols
4. Novel or improved characterization tools

A-2: Greener Advances in Catalysis and Energy (GrACE)

Catalysis is a critical component in US manufacturing, from fuel production to chemical synthesis for technologies and everyday products. In particular, new catalytic materials are imperative to the development of a green economy, including industrial catalysts and specially designed catalysts for biomass conversion that provide less waste, promote carbon sequestration, and reduce our dependence on foreign energy sources. A particular interest area are catalysts for converting waste to fuels and other chemicals, reducing waste streams,

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increasing fuel and chemical supplies, reducing carbon emissions and foreign oil imports.

AMES core capabilities in chemical and molecular sciences provide the necessary foundations for this initiative in experimental and computational design, synthesis and analysis of catalysts.

Goals – Continue to develop our leadership in predictive catalysis for a cleaner environment and more energy-efficient process streams, particularly using cooperative and 3D multifunctional catalysts. We will also find alternatives to rare-earth containing catalysts and leveraging capabilities in related efforts, such as Critical Materials Institute (CMI).

Focus Areas for Potential Funding (not exhaustive)

1. Electrocatalysis
2. Biomimetic catalysis
3. Computational tools for catalysis design
4. Development of capabilities through external partnering.

A-3: Primary Research Initiative on Magnetic Resonance of Solid-state for Energy (PRIMROSE): our Solid-State NMR initiative

The Ames Laboratory has a unique concentration of solid-state NMR expertise, with several PIs being recognized as “undisputed world-wide leaders in the field”. Towards our goals of establishing a center focused on solid-state nuclear magnetic resonance (NMR) science, we will address scientific drivers relevant to the mission of DOE, including:

- Provide DOE with a leadership position in enhanced solid-state NMR characterization methods, especially Dynamical Nuclear Polarization (DNP) NMR.
- Move the frontiers of solid-state NMR techniques in several areas, e.g., improved characterization of catalytic, complex biomolecular and inorganic materials.
- Take advantage of our unique concentration of solid-state NMR expertise.
- Enable others to access the AMES expertise in solid-state NMR characterization.

Goals – We will provide leadership positions with new world-class NMR capabilities to enable the design and discovery of new materials.

Focus Areas for Potential Funding (not exhaustive)

1. Dynamic nuclear polarization (DNP) SS-NMR development
2. Novel methods for analysis of catalysts and biomolecular materials