LDRD@SNL

JUNE 2015 SAND2015-5553R

Sandia National Laboratories
Laboratory Directed Research and Development

We welcome your questions, comments, and ideas for future LDRD projects to feature! Email your feedback to Marie Arrowsmith, mdarrow@sandia.gov

Probing Small-Molecule Degradation to Counter Enzyme Promiscutiy

Susan Rempe (PI), Juan Vanegas, Mark Stevens

An LDRD-developed drug therapy targets the molecules that feed cancerous cells while preserving healthy molecules, resulting in potentially much safer future treatment options.

Treating cancer effectively while minimizing medication effects on the patient has historically been challenging. Chemical therapies that "starve" cancer cells also end up depleting healthy cells. Sandia researchers, in conjunction with the University of Maryland and MD Anderson Cancer Center, have recently developed a drug targeted to treat acute lymphoblastic leukemia. This new treatment depletes asparagine, the molecule needed by cancerous cells to survive, while leaving glutamine—essential to cell health, and chemically similar to asparagine—untouched. The team performed high-resolution molecular simulations to introduce mutations into the enzyme-drug L-asparaginase type 2, which is commonly used to treat certain types of leukemia by depleting asparagine. Through this process, they were able to pinpoint the location in the enzyme's structure where a mutation would eliminate the drug's affects on glutamine. The drug (patent pending) is currently being tested on laboratory mice, and based on the results, human testing would follow. In addition to advancing cancer treatments, the techniques the team are developing could be used to assist with biodefense.

Read more in the Journal of Molecular Biology (July 1, 2015): *Catalytic role of the substrate defines specificity of therapeutic L-asparaginase (L-ASP)*.

Awards & Recognition for LDRD participants

Pavel Bochev was awarded an Ernest Orlando Lawrence Award for his pioneering theoretical and practical advances in numerical methods for partial differential equations.

In collaboration with two university professors, a Sandia team from the Exascale Grand Challenge received the Best Algorithms Paper Award at the 29th IEEE International Parallel & Distributed Processing Symposium. LDRD participants on the team include **Jonathan Berry**, **Branden Moore**, **Simon Hammond**, **Scott Hammert**, **Cynthia Phillips**, **Resnick**, and **Arun Rodrigues**.

Nanocomposite Barrier Films for Enhanced Thin Film Photovoltaic Stability

Erik Spoerke (PI), Margaret Gordon, Neil Sorenson

Sandia researchers are developing encapsulant materials to protect and seal solar cells from external elements and provide resistance against fires started by arc-faults.

Ensuring the long-term reliability and safety of cost-effective photovoltaic (PV) systems is critical to expanding the use of this technology. Failure or degradation of encapsulant coatings protecting sensitive PV materials and electronics from environmental moisture and oxygen is arguably the leading cause of PV degradation and failure. These failures affect reliable utility and introduce unacceptable maintenance and replacement costs. Sandia researchers are developing and evaluating a robust, low-cost, optically transparent, highly impermeable polymer-clay nanocomposite thin film barrier/encapsulant alternative.

Working with collaborators at Texas A&M University, the team has identified several nanocomposite thin film compositions that not only promise improved properties as a barrier to external elements (e.g., water and oxygen) that can degrade a solar cell, but also introduce a new resistance to fires started by arc-faults in damaged solar modules. Using a Sandia-developed arc-fault testing capability, initial evaluations of test samples treated with a nano-engineered thin film barrier have shown dramatically increased resistance to flammability under simulated arc-fault conditions. These results demonstrate the promise of this technology in additional areas concerned with protecting environmentally sensitive electronics (e.g., satellites and nuclear weapons). Continued testing and evaluation of these materials is expected to lead to improved understanding of this phenomenon and aid in the continued development of this potentially important new module encapsulant material.

LDRD PROJECTED BUDGET AND STATUS

FY15 Q3 $146 MILLION 380 PROJECTS FUNDED AT $144.5 MILLION

UPCOMING LDRD EVENTS

JULY 16
PIs/PMs notified of IAT sponsorship decisions

OCT 1 –OCT 15
PIs for accepted proposals submit Project Spend Plans

Sandia National Laboratories

Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

U.S. DEPARTMENT OF ENERGY