

NEWS

For Immediate Release

Contact: Katherine Kline
(304) 293-4611

Katie.Kline@mail.wvu.edu

Physics' Professor to Develop Detection of Explosives on Nanoscale

Morgantown, W.Va., July 17, 2007: One of the most important elements of effective homeland security is a quick response to explosives threats. These responses require sensitive explosives detection on a molecular level.

Dr. James P. Lewis, a Professor of Physics in West Virginia University's Eberly College of Arts and Sciences, received an EXP-LA (Explosives and Related Threats: Frontiers in Prediction and Detection) grant from the National Science Foundation totaling more than \$1 million to develop more efficient responding to explosives threats at home and abroad. Dr. Lewis joined WVU as part of WVNano, West Virginia's Nanoscale Science, Engineering, and Education (NSEE) Initiative. WVNano works across university boundaries to advance WV's research environment and diversify its economic base by cultivating and growing of discovery and innovation in targeted areas of NSEE. This award makes a major contribution to further building WVNano's research thrust in molecular recognition for security applications.

The project, "Collaborative Research: Exploiting Geometry and Chemistry at the Nanoscale to Selectively Preconcentrate Explosive Molecules," will develop Smart Nanoporous Preconcentrators (SNP) based on Metal Organic Frameworks (MOF). The distinguishing feature of this effort is its emphasis on using computational tools to obtain fundamental understanding of interactions between MOFs and target explosives. Dr. Lewis will collaborate with professors from the University of Tennessee at Knoxville, Jackson State University, and Oak Ridge National Laboratory to develop a preconcentrator technology that may enhance current chemical explosive detection capabilities. This will be achieved through computational analysis of suitable MOF structures, interaction between MOFs and explosives molecules, strength of binding, and diffusion. The PIs also intend to investigate effects of other factors critical for development of field technology: effect of temperature on MOF structure and associated explosives release rates, and potential contamination of SNP by non-explosive molecules.

The group will focus on detecting two explosive materials: RDX and TATP. RDX, or cyclotrimethylenetrinitramine, is the active component found in the plastic explosive C-4 and is widely used as rocket propellant. RDX is an energetic nitroamine—an explosive organic compound—which releases a large amount of energy upon decomposition, or breakdown.

TATP (triacetone, triperoxide, peroxyacetone) is organic peroxide that takes the form of a white powder and is sensitive to heat, friction and shock. TATP is known most recently for its presence in the London bombings that occurred on July 7, 2005. Dr. Lewis and his team will

also trace water and kerosene, a flammable hydrocarbon liquid, in internal surfaces of nanoporous media.

Dr. James P. Lewis recently joined the WVU faculty in 2006 after teaching and performing research at Brigham Young University. He developed computational simulations to understand the chemistry of explosives while he was a researcher at the University of Utah between 1998-2001. He earned his Ph.D. from Arizona State University in computational condensed matter physics. His research team has developed a code to predict the properties of a variety of materials ranging from DNA, semiconductors, carbon nanotubes, and many other materials. This simulation package, called FIREBALL, is being used by roughly 36 research groups worldwide.

The National Science Foundation funds specific research proposals that have been judged the most promising by a rigorous and objective merit-review system. This proposal was one of 28 (some of which are collaborative) proposals that were evaluated and ranked by a panel of experts assembled at NSF on May 17 and 18, 2007. Of the proposals evaluated, only three (3) one of which is this collaborative grant were ranked in the Highly Recommended category.

WVNano and its efforts building NSEE statewide receive primary support through the current NSF RII award with major matching contributions from the WVU, Marshall University, and the WV EPSCoR Office.

For more information, please contact Dr. James P. Lewis at James.Lewis@mail.wvu.edu.

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