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14. ABSTRACT
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Report Title

Report on Workshop on Targeting and Triggering from Molecules to Materials

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Number of Presentations: 0.00

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NAME
Total Number:

Names of other research staff

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Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See Attachment

Technology Transfer

Progress Report for the U.S. Army Research Office

Workshop on Targeting and Triggering from Molecules to Materials

Submitted by: S. Thayumanavan to Dr. Jennifer Becker (ARO); December 2014

This document reports on the proceedings and outcomes of the scientific workshop entitled 'Targeting and Triggering from Molecules to Materials'. We set out the following key points as the objectives of this workshop:

(i) To identify the knowledge gaps that are required to bridge the length and time scales of signal propagation from molecular to materials length scales.
(ii) To provide a cross-disciplinary forum for attendees to discuss the implications of developing new frontiers that will make fundamentally new advances in propagating molecular level changes to materials length scales.
(iii) To provide an opportunity for attendees to present their research results and identify partnerships to tackle this interdisciplinary problem collaboratively.

This workshop focused on bringing together scientists with complementary expertise to address the interdisciplinary and fundamental challenge of specifically targeting a molecular scale event, which can be seamlessly amplified to materials scale observation. Bridging the length scales and the time scales that molecular and materials level events and transformations provide is a grand challenge for the area of materials chemistry. This is the focus of this workshop.

The workshop was held at the University of Massachusetts Amherst campus on October 15, 2013. The workshop was organized and chaired by the PI. The PI also attended workshops and symposia on related topics held in Cambridge, England that was jointly organized by DSTL and ARO and an ACS symposium on stimuli responsive materials to produce this report.

Participants and Agenda:

We brought together a small set of participants with complementary scientific focus to address the important problem of targeting and triggering. It is understood that addressing this problem will require advances in supramolecular chemistry for the generation of advanced, responsive assemblies and participation of colloid and interfacial scientists to understand the origins of intermolecular forces as well as to characterize complex assemblies on surfaces and interfaces. Addressing this challenge will require us to take advantage of exciting advances in instrumentation that now make possible the dynamic imaging of supramolecular assemblies. Similarly, the development of such multiscale systems will require that molecular-scale assemblies be interfaced with engineered analytical processes and bulk materials, including materials with unique optical and electrical properties. Furthermore, these efforts must be aided, assisted and understood at a fundamental level through close collaboration with skilled theoreticians. Thus, a complementary, focused group of experts were brought together in this workshop to develop strategies to address this interdisciplinary problem.

The following agenda of the workshop includes the names, affiliation and the presentation topics during the workshop.

8:55 - 9:30 a.m. ***Introduction***

"Stimuli Responsive Nanoassemblies"

S. "Thai" Thayumanavan

Department of Chemistry, University of Massachusetts Amherst

9:30 - 10:00 a.m. ***"Targeting and Triggering using Liquid Crystals"***

Nicholas Abbott

Department of Chemical Engineering, University of Wisconsin Madison

10:00 - 10:30 a.m. ***"Precise nanoparticle and analyte positioning in liquid crystals"***

Juan de Pablo

The Institute for Molecular Engineering, The University of Chicago

10:30 - 10:45 a.m. ***Break***

10:45 - 11:15 a.m. ***"Particles and Macromolecules at Fluid Interfaces or Membranes: bending, binding and directing assembly."***

A. D. Dinsmore

Department of Physics, University of Massachusetts Amherst

11:15 - 11:45 a.m. ***"Theranostic Magnetic Nanostructures (Tx-MNS): Combining Non- Invasive Diagnostic Imaging with Targeted and Timed Therapeutic Delivery"***

Vinayak Dravid

Department of Materials Science and Engineering, Northwestern University

11:45 a.m. – 12:15 p.m. ***"Element- and Bond-Specific Soft X-Ray Spectroscopy of Soft Matter"*** Franz Himpsel

Department of Physics, University of Wisconsin Madison

12:15 - 1:15 p.m. ***Lunch and Informal Discussions***

1:15 - 1:45 p.m. ***"DNA, Peptides and Enzymes as Sense-response Components of Polymeric Nanomaterials"***

Nathan Gianneschi

Department of Chemistry & Biochemstry, University of California San Diego

1:45 - 2:15 p.m. ***"Dynamic Transmission Electron Microscopy"***

Nigel Browning

Chemical and Materials Sciences Division, Pacific Northwest National Laboratory

2:15 - 2:45 p.m. ***"Material Control through Peptide Design and Solution Assembly: Hydrogels to Hybrids"***

Darrin Pochan

Materials Science and Engineering, University of Delaware

2:45 – 3:00 p.m. ***Discussion of the Key Issues in Targeting and Triggering***

Summary of the Discussions:

Significant advances have been made over the past two decades in understanding the principles that underlie supramolecular chemistry. However, these advances have primarily focused on the equilibrium structures, leaving behind dynamics of the formation or transformation of supramolecular assemblies that respond to an environmental stimulus. In addition, systems that are predictably forced in and out of an equilibrium state are also of great interest. There will be a transformative impact, if one were to thoroughly understand the pathways by which these transformations occur and understand the effect of interfaces upon these pathways.

Also, molecular designs for generating changes in supramolecular assemblies are being consistently developed for classical stimuli. However, the design principles necessary for generating these changes in complex environments and unconventional stimuli are not currently available. Development of fundamental mechanistic understanding of triggering a discernible materials event in response to a specific change in the environment will have a large scale impact. If such strategies could be achieved in the complex environments, where the event is triggered based on very specific interactions between the material and the environment, then the impact will be even better. The lack of rational control over the design of supramolecular building blocks with precise chemical nanopatterns, and the associated absence of experimental techniques for measuring intermolecular forces encoded by such nanopatterns, has hindered past progress in this area.

Amplifying a response of functional supramolecular assemblies has impact in a variety of areas of interest to DoD. Examples include sensing in complex environments, materials that provide mitigation capabilities in response to an environmental variation, and self-healing responses to external stress. The need for materials that autonomously adapt and respond to changing environmental cues is tremendous. This type of targeting and triggering responses are currently impossible in synthetic materials, but ubiquitous in nature. Propagating molecular scale, selective recognition events through large areas and over multiple length scales are absolutely necessary for such systemic changes in materials properties. A fundamental understanding of dynamic, responsive systems far from equilibrium is an unmet need in chemistry, physics and engineering.