FEWS: Food-Energy-Water Systems Challenging Chemists in the 21st Century

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Preface

What are the avenues for chemists and chemical engineers in the 21st century to address critical fundamental scientific and technological challenges at the food, energy, and water nexus? How will chemists team in unprecedented ways with other disciplines to address interdisciplinary scientific questions related to this nexus? This workshop report describes a collective vision to address these two pressing questions with input from an interdisciplinary group of leading academic and industrial scientists and engineers to envision the critical role for chemists at the rapidly emerging nexus of food, energy, and water. The report is based on diverse input, including chemists, life scientists, environmental engineers, chemical engineers, agricultural community leaders, and soil scientists, to create a comprehensive vision for the chemical community. Grand challenges range from sensors for ensuring efficient water utilization and purification to educating the next generation of interdisciplinary chemists for impact on this critical field. This report identifies the top grand challenges as identified and prioritized at the workshop. The workshop comprised ten oral presentations to nurture discussion, and in-parallel working groups allowed small teams of scientists and engineers to clarify the challenges and provide examples of specific fundamental questions of science. This report is not intended to be comprehensive in content, but the report exemplifies challenges where fundamental advances in chemistry will be critical to ensure broader impact. ***It was clear that this nexus demands a new cadre of scientists who engage with interdisciplinary partnerships in an unprecedented manner.***

This report will catalyze discussion and present potential opportunities for chemists in the coming decade, consistent with crosscutting initiatives at the National Science Foundation. The chemist plays an important role in team tackling these challenges, enabling next generation technologies, and training the next generation workforce. Although chemists have successfully pursued the energy-water nexus over the past decades, the addition of the food and agriculture lens imposes new challenges for the chemist and the opportunity to engage in active partnerships with new scientific fields from smart farming to soil science. Agriculture accounts for 80% of human water use, and our attention to water and nutrient availability will be critical in the future.

Now is the time for chemists to nurture unprecedented partnerships and initiate an interdisciplinary discourse that leads to fundamental science and engineering necessary for technologies of the future to address the food-energy-water global grand challenge.

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I. Executive Summary

This report defines grand challenges as collectively identified with interdisciplinary participants of the Innovations at the Nexus of Food, Energy, and Water Systems (INFEWS) workshop. This report describes the role of fundamental advances in chemistry and chemical engineering to address these challenges, from analytical chemistry to surface science and synthetic purification membranes. The role of chemists and chemical engineers at INFEWS intersections is crucial to the development of sustainable solutions to address these grand challenges. This report will emphasize connections to NSF priorities, including data analysis and infrastructure, computational chemistry-guided experimental research (see the National Strategic Computing Initiative), and the Materials Genome Initiative (see the NSF DMREF program). This report defines the central role of the INFEWS theme across many disciplines, thus recommending a continued crosscutting research investment in fundamental science and engineering for addressing this global imperative.

Grand Challenge 1: Promoting collaboration between chemists, other stakeholders, and scientists traditionally engaged in agricultural, water and energy enterprises: Establishing and nurturing interactions between chemists and soil scientists, environmental engineers, agriculturalists, physicists, and biologists is paramount to the generation of feasible solutions for INFEWS grand challenges. The development of shared workspaces, such as those partnerships between industry, government, and academia to collaborate is vital to the understanding of these global challenges. In addition, the collaboration between scientists goes beyond a "divide and conquer" system and must include the training and interdisciplinary understanding of each discipline related to a grand challenge.

Grand Challenge 2: Educating future INFEWS professionals and fostering public understanding of food, water, and energy issues and emerging chemical technology: Education of the next generation of scientists must begin at an early age, with grand challenges at the INFEWS interfaces addressed beginning in public elementary and high schools. Furthermore, agriculturists and politicians require education surrounding these grand challenges in a sustained fashion over the next decade. Developing and implementing solutions now will lay the groundwork for the future tackling of rapidly emerging INFEWS issues.

Grand Challenge 3: Improving water use efficiency in agriculture and industry: The first essential step to a sustainable water supply is the development of conservation strategies and techniques to prevent drought and water shortages. The majority of water use is devoted to agriculture, and a significant amount of this water is overused, resulting in runoff. The development of solutions for targeted water delivery with minimal waste will not only improve soil quality but also aid in conservation of water resources.

Grand Challenge 4: Fundamentally understanding structure and transport in complex porous and non-porous materials: Significant earlier attention describes the transport of water and energy at the macroscale, however, the mechanism of water absorption in soil or how various molecules transport and interact within multi-component systems remain relatively unexplored. The first question is the understanding of the structure and composition of these complex systems; as an example, soil is composed of metals, minerals, and microbiota, much of which remains poorly understood. Furthermore, how these transport phenomena change as a function of time is a crucial aspect to addressing these questions.

Grand Challenge 5: Developing an infrastructure of measurement tools for analyzing complex systems: While many researchers are addressing chemical transport mechanisms, the development of new analytical tools to evaluate complex mixtures of materials are necessary. Instruments with high sensitivities and the ability to separate small molecules are crucial to understanding the transport and transformation of diverse compounds through both soil and aquatic systems.

Grand Challenge 6: Design and characterization of macromolecular and supramolecular materials to improve water efficiency/quality and food production: Polymer science is at the forefront of new materials for solutions to INFEWS problems, including water purification membranes, food packaging, and controlled release fertilizers. "Smart" materials, such as those that can self-detect and materials to aid in the determination of food aging are at the forefront of the INFEWS research vision.

Chemists and chemical engineers must consider life cycle analysis for the successful translation of new technologies, and in-parallel cost considerations are essential for successful translation and scale-up. Proposed innovations

must include a translational lens of the "laboratory to the land" to ensure broader impacts.

Grand Challenge 7: Revealing surface chemistry and interfacial phenomena important to the INFEWS nexus: Interfaces and surfaces between systems are inherent to many scientific questions at the agricultural interface. The interaction of surfaces with their surroundings, such as water purification membranes with unclean water and soil with the surrounding air and water, are crucial to both the understanding of how these problems originate as well as the development of new solutions.

Grand Challenge 8: Understanding chemical processes in complex mixtures: All chemical reactions in INFEWS systems happen in complex mixtures, such as the transformation of drugs in aquatic systems or reactions between metals and nutrients found in soil. Understanding how these complex systems affect chemical reactions, whether to inhibit or stimulate them, is vital to understanding how many of these global issues develop. With a greater understanding of how many chemical species interact comes the opportunity for new and sustainable solutions.

Grand Challenge 9: Protecting water resources by targeting the delivery and understanding the fate and transport of bioactive compounds: Many water supplies are contaminated by a large variety of chemical substances, with the most common and prevalent one being fertilizers and their products. The development of targeted fertilizers to reduce or eliminate the chemical waste introduced to the water supply and the study of how these fertilizers enter the water supply is vital to the preservation of precious water resources.

While these grand challenges are in no way fully inclusive of all the issues facing INFEWS, they provide a comprehensive guideline to address those challenges that are both the most vital to intervening in an impactful way and feasible to address with the current infrastructure provided to scientists. A fundamental understanding of how INFEWS interact and how many of these issues arise is a vital piece to the development of sustainable solutions to these problems. This report addresses these grand challenges in more detail as well examples of specific research programs.

II. Introduction and Background: Challenges for Science & Engineering, Education, and Policy/Financial Models for Societal Impact

Humanity is reliant upon the physical resources and natural systems of the Earth for the provision of food, energy, and water. It is becoming imperative that we determine how society can best integrate across natural and built environments to provide for a growing demand for food, water, and energy while maintaining appropriate ecosystem services. Factors contributing to stresses in the food, energy, and water systems (FEWS) include increasing regional, social, and political pressures as result of land use change, climate variability, and heterogeneous resource distribution. These interconnections and interdependencies associated with the food, energy and water nexus create research grand challenges in understanding how the complex, coupled processes of society and the environment function now, and in the future. There is a critical need for research that enables new means of adapting to future challenges. The FEW systems must be defined broadly, incorporating physical processes (such as built infrastructure and new technologies for more efficient resource utilization), natural processes (such as biogeochemical and hydrologic cycles), biological processes (such as agroecosystem structure and productivity), social/behavioral processes (such as decision- making and governance), and cyber elements. Investigations of these complex systems may produce discoveries that cannot emerge from research on food or energy or water systems alone. Chemists must employ this synergy using a lens of sustainability that will enable innovative science and engineering pathways to solve the challenges of scarcity and variability.

The increased demands for fresh water for crops/livestock and energy production will significantly add to the current stress on non-renewable water resources. Estimates predict that seven billion people in sixty countries will experience water scarcity by 2050 at current rates of water usage. This will place additional stress on both food supplies and energy consumption rates. These needs necessitate scientific and technological innovations that will address global problems that center on fresh water.

Developing new water supplies has historically been society's answer to growing demands, particularly in the developed world, but in recent years the costs of new supplies and concerns over their environmental impacts have led to greater focus on "managing" (i.e. reducing) demand and reconsidering how existing supplies are allocated across uses (e.g., urban, agricultural, environmental). In both cases, it is the "institutions" governing the allocation of water, that is the rules and decision making frameworks that surround people's choices, that have a tremendous impact on who uses water and how much. Given the relative abundance of water in most places, robust water-related institutions are often underdeveloped or at least underemployed. Nonetheless, the rising financial and environmental costs of new supplies have provided greater motivation for institutional innovation and subsequent implementation. This is visible in water use and supply development trends at both the local and regional scales, creating more complex decision making scenarios in which both structural and non-structural approaches to meeting future water demands must be integrated. These strategies require sophisticated approaches for allocation of existing resources particularly during drought times. In addition, these strategies require the integration of approaches with new infrastructure development.

As we face a world population expected to reach 9.5 billion by 2050, we will continue to stress our basic resources of soil, water, and air. To feed 9.5 billion people will require application of proven technologies and development of new technologies. This must be done while enhancing the quality of life, especially in developing countries, of millions of rural residents that depend on agriculture for their livelihoods. At the same time, we must minimize environmental impacts and avoid ecosystem degradation.

The integration of the soil, water, and plant component of an agroeco-system will create sustainable food production. To create this sustainable future, fundamental science and engineering is necessary. For a chemist and soil scientist working together, we must have a clear understanding of how technologies, both emerging and existing, affects the biological/biochemical, chemical and physical properties of the soil-water-plant agroecosystem to produce food, feed, fiber, and fuel. Soil physics is the study of soil physical properties and processes for the management and prediction of natural and managed ecosystems. Soil

physics deals with the dynamics of physical soil components and their phases as solid, liquids, and gases. Soil chemistry is the study of the chemical characteristics of soil. Mineral composition, organic matter, and environmental factors play critical roles on soil fertility. Soil biology/biochemistry is the study of microbial and faunal activity and ecology in soil and their related biochemical processes.

Soil is the “switching yard” of the global cycles of nutrients and water. Of particular importance are the cycles of carbon and nitrogen as these two nutrients have the greatest impact on both crop production and environmental, e.g. water, quality. In many regions of the world, the availability of nutrients limits food production, leading to soil degradation such as erosion, because of poor soil cover. In other areas of the world, the problem is application of excess nutrients that runoff of agricultural fields and impact environmental quality. Chemists in the 21st century must strive to understand how to improve the use efficiency of nutrients. Future research must focus on applying basic principles of physics, chemistry, and biology/biochemistry to our soil resource base. Timing for this attention is critical, otherwise history has recorded for us that civilizations will fall.

III. Fostering New Interdisciplinary Teaming at the INFEWS Intersection

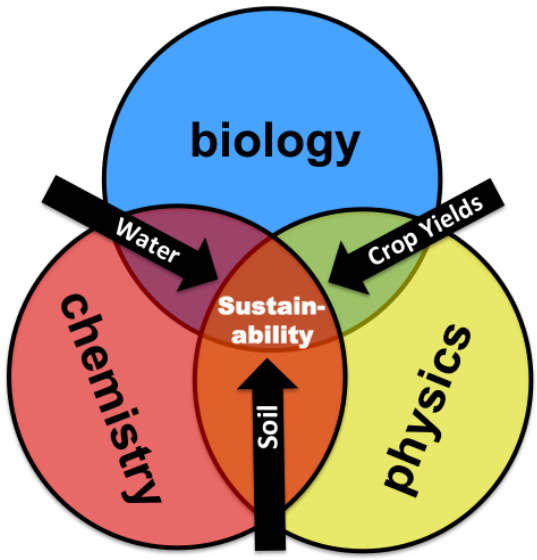

Figure 1: *Interdisciplinarity is necessary to achieve sustainable solutions to INFEWS grand challenges. Chemists must partner in unprecedented ways with soil scientists and agricultural life scientists.*

Materials innovation will enable new technologies. New ideas, concept demonstration, and dissemination of the information are indeed an important step in the innovation cycle. But with the grand challenges facing the world, for example in the food-energy-water "system", there should be a more multidimensional approach to "innovation that matters", i.e., how we can improve the pace of development and ultimately get more significant, breakthrough solutions to the world to impact communities, as illustrated in Figure 1.

Grand Challenge 1: Promoting collaboration among chemists, other stakeholders, and life scientists traditionally engaged in agricultural, water, and energy enterprises

One of the most striking observations from the workshop was the fact that scientists and engineers in the various disciplines have been insulated from each other making important discoveries that ultimately need other disciplines to explain fully. Side-by-side research efforts have been conducted with minimal, if any, co-knowledge. As a result, findings have been accurate, but misaligned, and often impractical for implementation by the broader agricultural community.

Fascinating and challenging science, engineering, and life happen at interfaces, e.g., solid/liquid interfaces such as water passing through a plant root cell wall or synthetic polymer membrane or water restrained by a natural riverbank or engineered dam. Likewise, fascinating and challenging advances in science, engineering, and life occur at interfaces between the disciplines. Interdisciplinarity is the combination of knowledge from more than one academic, scientific, or artistic discipline. Interdisciplinary research works to tackle complex issues that a single-discipline is inadequate to address because the knowledge required crosses traditional physical, biological, economic and social disciplines and requires experts and novices to work at the interfaces between them.[2,3]

Interdisciplinary solutions thus combine diverse sources and levels of expertise. Two or more parties working together to solve the same challenge may not have an in-depth understanding of each other's science. For this reason, interdisciplinary work requires particular skills, mindsets, and attention to establishing common ground. The first steps in establishing interdisciplinary projects are crucia.[4] "Projects did not succeed as well as they might have because they did not facilitate 'enabling conversations' from the outset and because they lacked coherent leadership".[3] Consequently, interdisciplinarity hinges on communication.

There is a critical need for scientists (physical, biological, and social) and engineers to form interdisciplinary teams to evaluate and implement solutions for global food, energy, and water challenges and to do so with consideration of health, safety, and public perception. Increasingly, researchers and practitioners must give their attention to multidisciplinary views, e.g., chemistry, biology, physics, economics, social sciences, and engineering, to produce an interdisciplinarity that is necessary for contemporary problem-solving at the nexus between disciplines for the benefit of society.[5] Ultimately, the interdisciplinary knowledge and experience gained within the INFEWS community will influence global food, water, and energy security for the expanding human population.

To foster this new interdisciplinary teaming within INFEWS, the workshop recommends that chemists:

- Communicate competently to peers and the public
- Learn to think abstractly, dialectically, creatively, and holistically
- Research beyond our traditional comfort zones and with new colleagues
- Maintain adaptability and flexibility while exploring interdisciplinary solutions
- Develop and work toward a common goal
- Respect and appreciate interdisciplinary team members
- Maintain humility and tolerate ambiguity

Recent data indicates that globally, interdisciplinary research is growing, gaining influence [5,6] and gaining funding.[3] The INFEWS community will contribute to this interdisciplinary growth in order to resolve complex issues that face society.

Creating "playgrounds" for open interdisciplinary interactions: The collaboration between industry, academia, and government to create analytical centers for scientific discovery has led to numerous favorable collaborations and scientific breakthroughs. These centers are common for the evaluation of technologies such as nanotechnology, but remain absent for the emerging INFEWS interface. The development of such centers that contains specialized analytical tools for the analysis of INFEWS samples would not only allow for additional characterization of these materials, but foster collaboration between academia, industry, and the government.

Creating interdisciplinary degrees and expanding opportunities for training: Chemists must envision new mechanisms for training, uniquely allowing chemists to explore intersections with life scientists and agricultural disciplines. This should occur from the elementary level through the graduate level, emphasizing opportunities for innovation, entrepreneurship, and discovery for undergraduates. Departments of Chemistry should consider novel interdisciplinary graduate education programs that provide sufficient flexibility to explore agricultural disciplines. Collaborating with industry e.g. employing many federal programs such as the NSF GOALI program will ensure career awareness for students and infuse needs validation to research programs. Accelerating societal impact is a critical metric for success.

IV. Educating Stakeholders and the Next Generation INFEWS Workforce

The workforce of tomorrow continues to change rapidly and institutions of higher education must prepare our undergraduate and graduate students for future employment opportunities. The knowledge, skills, and abilities (KSA) for success will continue to evolve. This challenge will focus on interdisciplinary and transdisciplinary thinking, the professional development needed for undergraduate and especially graduate students to successfully transition to the workforce and the ability to communicate effectively. The food-energy-nexus exemplifies the necessity for interdisciplinary training with keen attention on societal impact. Water plays a critical role in energy and agriculture, and as our population continues to grow, the innovator will need to be able to communicate in multiple disciplinary languages resulting in new interdisciplinary languages of science. New degree programs will emerge in the next decade to provide a mechanism to train the next generation of FEWS scientists and engineers. Interdisciplinary education and problem solving is no longer a paradigm at leading institutions, it will be an expectation. In addition to interdisciplinary thinking to tackle complex global problems, business and interpersonal skills for entrepreneurship will be a critical component of the future graduate's portfolio.

A sense of community is often defined as a feeling of fellowship that emerges as a group shares common attitudes, interests, and goals. A new FEWS community will evolve from (1) a shared vision for the global needs for food, energy, and water, (2) common awareness of potential interdisciplinary technological solutions, (3) a passion for volunteerism in a larger community, and (4) an understanding of the necessary networks and societal mechanisms that are essential to navigate as a community leader.

Grand Challenge 2: Educating future INFEWS professionals and fostering public understanding of food, water, and energy issues and emerging chemical technology

Research performed in the lab will not generate significant changes at the INFEWS interface without the dissemination of this research to the water and agricultural community. Communication between scientists and the public is essential to the proper dissemination of new research findings. Most importantly, the dissemination of information to the agricultural community on strategies for irrigation and soil health will significantly improve both the quality of soil and nutrient delivery and the preservation of water sources. This dissemination will involve training programs and informational literature that is available to the agricultural community free of charge or at a low cost. The utilization of low-cost solutions is essential for these resolutions to be widely implemented throughout the agricultural community.

Next Generation INFEWS Workforce

Graduate Student: Graduate institutions will need to develop and enable collaborations in related disciplines that leverage the strengths of diverse faculty interests and expertise. Faculty will need institutional support to teach, mentor, research, and publish with students in these interdisciplinary teams.

Undergraduate Students: It will be critical for students in traditional physical and biological science programs (biology, chemistry, and physics) to achieve formal exposure to the systems and skills used in the environmental and agricultural fields. Engaging undergraduate students in both the content and skills will provide pipelines of interest to graduate schools and industry. There is a need to develop INFEWS curriculum modules and laboratory experiments (polymers/membranes, surface/interface chemistry, soil chemistry, watershed science) at the undergraduate level with faculty teams trained to deliver this curriculum.

In addition to institutionalized education on issues surrounding INFEWS, the development of a wide-scale design challenge to meet some of these issues is necessary. Similar to those found in the biomedical field, design projects that challenge students to create zero-energy, cost effective solutions to grand challenges would not only involve the next generation of the INFEWS workforce, but also provide innovative solutions across disciplines to these grand challenges. As an example, the development of sensors to aid workers and end users on the quality of food as it ages would require students in agriculture, engineering, and sciences to come together to generate meaningful solutions to this grand challenge.

V. Improving Water Use Efficiency in Agriculture and Industry

Traditionally, scientists and engineers consider energy and water issue independently. However, water and energy are interdependent. Energy production and generation require water, as in the case of power plants, which require substantial quantities of coolant water for generating electrical energy. In oil and natural gas production, for every 80 million barrels of oil produced per day 250 million barrels of produced water are generated, defining the water to oil ratio greater than 3:1. Similarly, water pumping, treatment, and distribution require energy. In the future, threats to the production of energy will potentially result from limited water supplies. This threat increases with population growth and the associated increase in water demand. Competing demands for water supply by the industrial, agricultural, and domestic sectors are also affecting the availability of this essential resource.

Based on this scenario, there is an urgent need to use non-traditional waters to increase the availability of water resources for generating electricity without affecting other important sectors. Non-traditional waters include brackish groundwater and produced water with elevated levels of total dissolved solids (TDS) and/or metals. Waste heat is also present in some non-traditional waters, which are potentially recovered and reused.

Desalination of non-traditional waters using current membrane separation technologies such as reverse osmosis (RO), become a challenge. One of the major limitations that RO faces is the excessive energy cost of desalinating water with concentrations higher than 10,000 mg/L. Additionally, the accumulation of mineral salts on the surface of the membrane poses a threat to the life span of the membranes, causing fouling, scaling, and ultimately damage of the membrane. New emerging technologies, such a forward osmosis, electrodialysis metathesis, and membrane distillation, may face similar limitations as RO due to the lack of membranes resistant to high TDS concentrations and scaling.

Research challenges in membrane technology for desalination include new membrane materials, based not only on traditional polymers, but also on nanomaterials such as graphene, graphene oxide and composite nanomaterials. The recovery of waste heat from non-traditional waters with an increase in the availability of pure water will decrease the energy cost of emerging technologies.

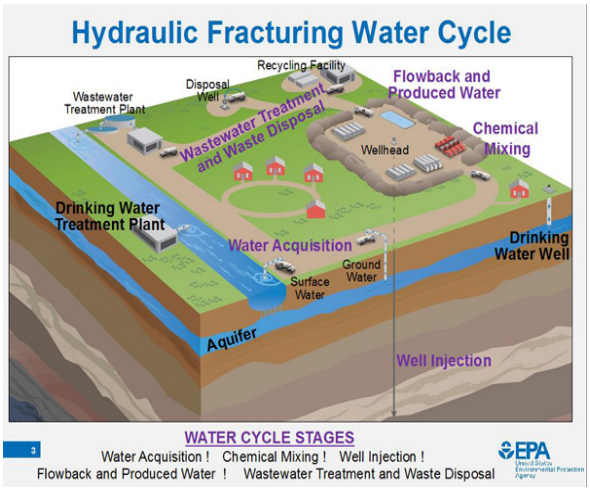

Figure 2: *US EPA – water cycle in hydraulic fracturing.*

Grand Challenge 3: Improving water use efficiency in agriculture and industry

Translating fundamental understandings of soil chemistry to maintain soil health and reduce irrigation volume: The translation of basic scientific investigations of soil chemistry, compositions, and reactions to the preservation of soil health is essential to solving many agricultural problems. This includes nutrient and water diffusion through soil as well as optimal times and amounts of water used for irrigation. The reduction of water volumes used for irrigation will aid both water conservation and preservation of soil health. Runoff and soil erosion is common with the overuse of water and changes associated with soil. The understanding of how water diffuses through soil, how soil composition changes over time, and the effect of microbiota and metal compositions will affect these translational results. Discovery of artificial soils, both for examination of fundamental soil properties and potential solutions to soil erosion, is necessary for successful agricultural intervention.

Drought resistant agricultural structures with water management in Biosystems: Participants in the INFEWS workshop identified repeatedly the wastefulness of water use in agriculture, because of a historical culture of treating water as an essentially limitless resource.

However, there are now numerous documented local- to regional-scale water shortages and cases where the over-application of nutrients, herbicides, and pesticides has led to a degradation of soil and water. Agriculture needs tools and technologies to improve irrigation efficiency, the application of pest control chemicals, and the mitigation of the transport of non-point pollutants. Wireless sensor networks are an emerging and promising technology to accomplish the goal of improved water management. Challenges include reducing cost and increasing robustness and detection efficiency of the sensors. Furthermore, difficult decisions remain concerning the type of crops grown, versus the climate, economic margin, and water supply, particularly in water-short regions of the world. In both industrial water use (see below) and in agriculture, education and training of the operators (in industrial use) and growers (agriculture) in field measurement techniques and the value/purpose of these data is also key to success.

The nexus needs improved characterization of municipal and industrial wastewaters, (e.g., produced/flowback waters from unconventional oil & gas wells). Recovering and recycling wastewater presents a number of daunting technical challenges, including removing contaminants of concern, salts, and pathogens—all by highly efficient and energy effective means. For example, in terms of improving water use efficiency (reuse/recycling/conservation) and disposal practices (reducing risk), better knowledge of systematic changes in the chemistry of unconventional oil and gas produced water as a function of time or volume produced would be of great use, particularly on the organic chemistry and trace metals sides. Challenges include identifying complex organic molecules, and quantifying potentially toxic trace metals (at ppb or ppb levels) that exist in brines with total dissolved solids (TDS) often-exceeding 20%. Laboratory methods serve as a baseline to develop a set of field measurements or the development of sensor networks. These data may potentially inform the application of appropriate membrane technologies for various fractions of the wastewater, saving cost, improving water use/recycling efficiency, and potentially reducing risk.

Figure 3: *Catchment runoff, including agricultural runoff. http://www.jointheevolution.ca/blog/2009/06/22/the-water-that-flows-part-1/*

On a broader scale, water networks for large agricultural (see Figure 3) and industrial field systems (see Figure 2: US EPA figure for a hydraulic fracturing water cycle example) are complex, and it is practically impossible to track the fate of each drop of water. However, understanding the mixing of various waters that occurs in holding tanks, pipelines, irrigation networks, reservoirs, holding ponds, in the subsurface, and due to phenomena including evaporation and precipitation has impacts on the chemistry (and microbiology) of these waters. There are specific targets for water chemistry (and microbiology) in operations, and thus a better understanding of the water cycle would ultimately feed into understanding the chemistry and microbiology (e.g., biofouling) that occurs in these systems. In such large distributed water networks, developments of more advanced sensor networks (indeed rudimentary ones are in current systems) are necessary.

VI. Fundamental Understanding of Transport/Diffusion in Complex Media

Water purification membranes are essential technology for the generation of clean waters for human use. Since the inception of FT30-interfacial polyamide chemistry by the late John Cadotte, there has been significant interest to improve both energy and separation efficiency for reverse osmosis (RO) operations from a membrane chemistry standpoint. The polyamide membrane is not soluble in common organic solvent and neither is easy to apply conventional analytical techniques. In addition, the polyamide layer is a part of three layer composite structure and is difficult to delaminate the membrane. As a result, development of structure-property relationships has been a challenge in the last couple of decades. In addition to polyamide membranes, surface characterization of water purification membranes and property changes over time is also a largely unanswered question.

In the last few years, leveraging Dow's strong analytical capabilities and blending with Dow Water & Process Solution expertise, it has been possible to achieve a true fundamental structure-property relationship of the polyamide RO membrane. In depth characterization of polymer composition, morphology, topology and post gel properties coupled with fundamental transport and structural modeling led to a breakthrough in membrane chemistry innovation. The breakthrough membrane chemistry resulted in lowering the energy requirements for brackish water RO operations by 35% and at the same time reduced salt passage by 40% over industry standard products. This breakthrough technology will result in the production of over 15 trillion cubic meters of clean water (the volume of over 6 million Olympic-sized swimming pools), while saving over 2 billion kilowatt-hours of energy and over 1.5 million metric tons of CO_2 emissions. At the same time, the technology targets several other applications to improve productivity, reduce footprint and in overall improve the quality of the water.

Membrane technology is at the present one of the best alternatives to treat salinity water for water augmentation with low energy footprint compared to the energy-intensive thermal desalination processes. RO has found a market as the best available membrane desalination process. Earlier advances have increased the efficiency of the RO process; however, an important limitation of the process is fouling of the membranes. Novel technologies such as forward osmosis (FO) and membrane distillation (MD) are advancing as alternatives to treat new generation of impaired waters, including high-salinity waters generated during the hydraulic fracturing process used to extract shale gas.[7] One of the grand challenges that RO, FO, and MD faces is the development of membranes resistant to the fouling effect that minerals and other components present in the water cause to the surface and internal structure of the membranes during the separation process. Concentration polarization caused by minerals accumulation is responsible for the reduction of permeate flux and water quality, and increase of energy required to keep the process running. These components may include scale products such as calcium sulfate, barium sulfate, and strontium sulfate, organic components such as dissolved and suspended organics, as well as naturally occurring radioactive and heavy metals. They may be present individually or forming complex matrices that accumulate on the membrane surface and ultimately cause damage of the membrane. Chemists are need to probe the structure and properties of membranes that are resistant to fouling effects; this requires an in depth understanding of the transport mechanisms of single components, binary and complex mixtures across the membrane, but also of the mechanisms accompanying the concentration polarization caused by these complex transport mechanisms. New generation of membranes will be facing the complexity of reactions taking place at the surface of the membrane, where not only individual components and mixtures will be dynamically reacting but also complex process and operating conditions influence the kinetics and interactions of such components and therefore the overall membrane transport mechanisms.

Grand Challenge 4: Fundamentally understanding structure and transport in complex porous and non-porous materials

Water and ion movement through soil, polymers, and heterogeneous structures: Soil wettability and the corresponding ion and water movement through soils is an ongoing problem in agriculturally rich regions. The development of predictive modeling and the study of the interplay between water and salt movement through soil to

predict soil health is needed to fully elucidate the effects of irrigation, drought, and other disastrous events on the soil.[8]

Furthermore, how these interactions influence the development of humus and the interaction with the microbiota are all crucial aspects to understanding how water moves through the soil and how this changes over time. Mathematical modeling of soil systems is essential to predicting the movement of these ions and water through the soil matrix, as demonstrated in Figure 4.

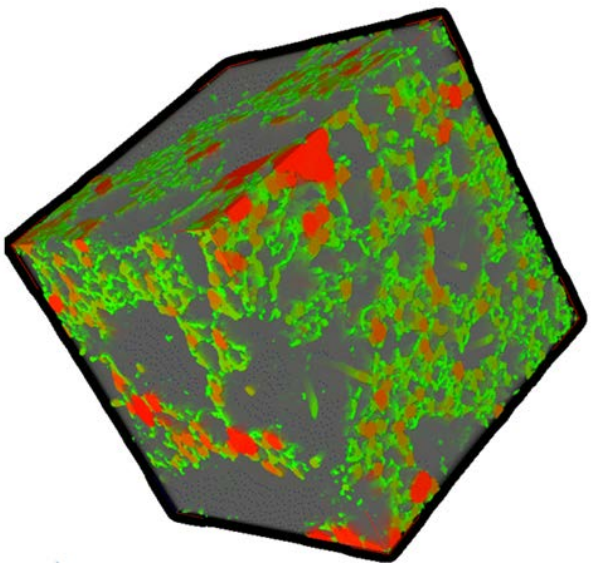

Figure 4: *Inter-aggregate pore space within an inscribed cube (1cm^3) of soil representing supply paths of oxygen and location of fast flow and transport processes. Grey: diffusive domains, Green: voids, Red: interconnected pores >30 microns.*

Understanding energy needed for water and ion movement through structured membranes (fouled and pristine): The interplay between energy and water is a profound one; as water purification membranes are fouled, the amount of energy required to move water across the membrane changes significantly. Both the mechanism of fouling and energy requirements change as a function of time is essential to predicting the lifetime and cost of water purification membranes.[9] The evaluation of how the nanostructure of the membranes changes the water and ion transport across the membrane is essential to the design of new membranes with greater water permeability, increased salt rejection, and fouling prevention. With each membrane, the energy required to move water and salts across the membrane would change as a function of fouling.

Predictive modeling and computational simulations across different length scales: While water movement through porous media occurs generally at the micron-length scale, the effects of water movement and diffusion through soils is a macroscale problem, leading to issues of nutrient uptake in plants and significant runoff. Developments in modeling strategies that can predict and evaluate these effects on both the micro and macro scale will attempt to address these concerns. An additional example where both the micro and macro scale length effects are crucial is in water purification; the movement of water and the elimination of ions with a water purification membrane are necessary to understand the water purification process. However, in addition to this small scale, water movement across pipes from the treatment plant to homes (this is especially crucial in California, which transports water across large length scales) is necessary to understand how the quality of the water changes as a function of time and to determine the energy costs of the system.

Probing "space" in chemical, macromolecular, and soil structure: New techniques are needed to explore the 3-dimensional free volume structure of polymers of interest for membrane applications. This free volume structure has a characteristic length scale at angstrom dimension, and it is critical for determining selectivity and rates of transport in membrane systems. The current state-of-the-art for characterizing free volume is positron annihilation lifetime spectroscopy (PALS). PALS measures the bulk free volume properties of polymers, and is not presently capable of probing the local free volume structure in materials. New techniques, either experimental or molecular dynamics simulations, are needed to develop fundamental relationships between polymer chemistry, structure, and free volume. An ideal experimental technique would be able to probe angstrom-scale features without disturbing the chemical or structural environment of the polymer.

Developing new analytical techniques for real-time measurement of transport in relevant environments: Analytical tools to evaluate INFEWS transport in real-time will fully elucidate the pitfalls and advantages of current technologies. For example, real-time evaluation of fouling on water filtration membranes would provide insight into the mechanisms of biofouling and the dynamics of water transport across the membrane. As another example, the real-time monitoring of the transport of nanomaterials and contaminants through aquatic systems, as seen in Figure

5.[10] The development of these analytical tools at a favorable cost is essential to the understanding of the complex interplay between these dynamic processes.

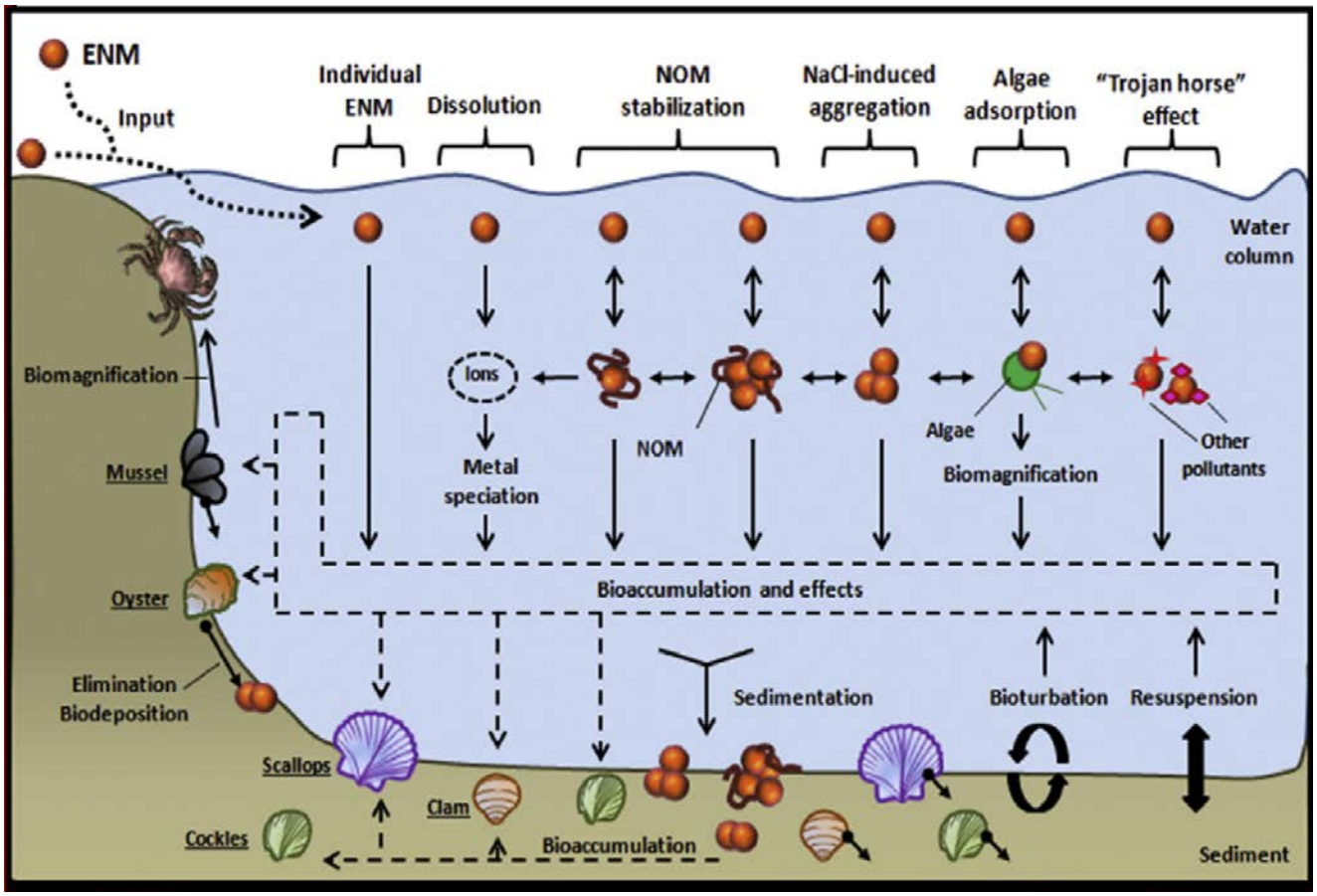

Figure 5. *Potential fate and behavior of engineered nanoparticle contaminants to water quality and aquatic life.*

VII. Instrumentation Infrastructure, Computational Modeling, and Data Analytics

Water is precious resource for every country. Water purity is also a resource of considerable value. Often surface waters, rivers and streams, as well as the water table have become complex mixtures of metals, pesticides, herbicides, pharmaceuticals, and polycyclic aromatic hydrocarbons often along with microbial pollution. The diversity of pollutants in water continues to expand. Some pollutants are caused by desorption from natural minerals and rocks; nonetheless, these pollutants can be quite toxic. Pollution caused by anthropogenic sources such as excessive agricultural fertilization and the heavy use of herbicides and pesticides impacts the quality of river and stream water. In addition, trace levels of pharmaceutical compounds are increasingly prevalent, especially in urban environments. Furthermore, fracking activities across the country potentially pollute ground water. This section will review the variation of the types of pollutants and the observed range of pollutant concentrations.

Advanced state-of-the-art analytical measurement techniques for these pollutants are critical. Based on a careful analysis of the information provided, innovations to provide sustainable water sources for plant and animal life are important considerations. Figure 6 illustrates the unifying role of computational modeling and data analytics to tackle big data obtained from diverse sectors of water management. Advances in analytical tools for real-time monitoring will provide unprecedented access to large data sets to more accurately manage water use in agriculture.

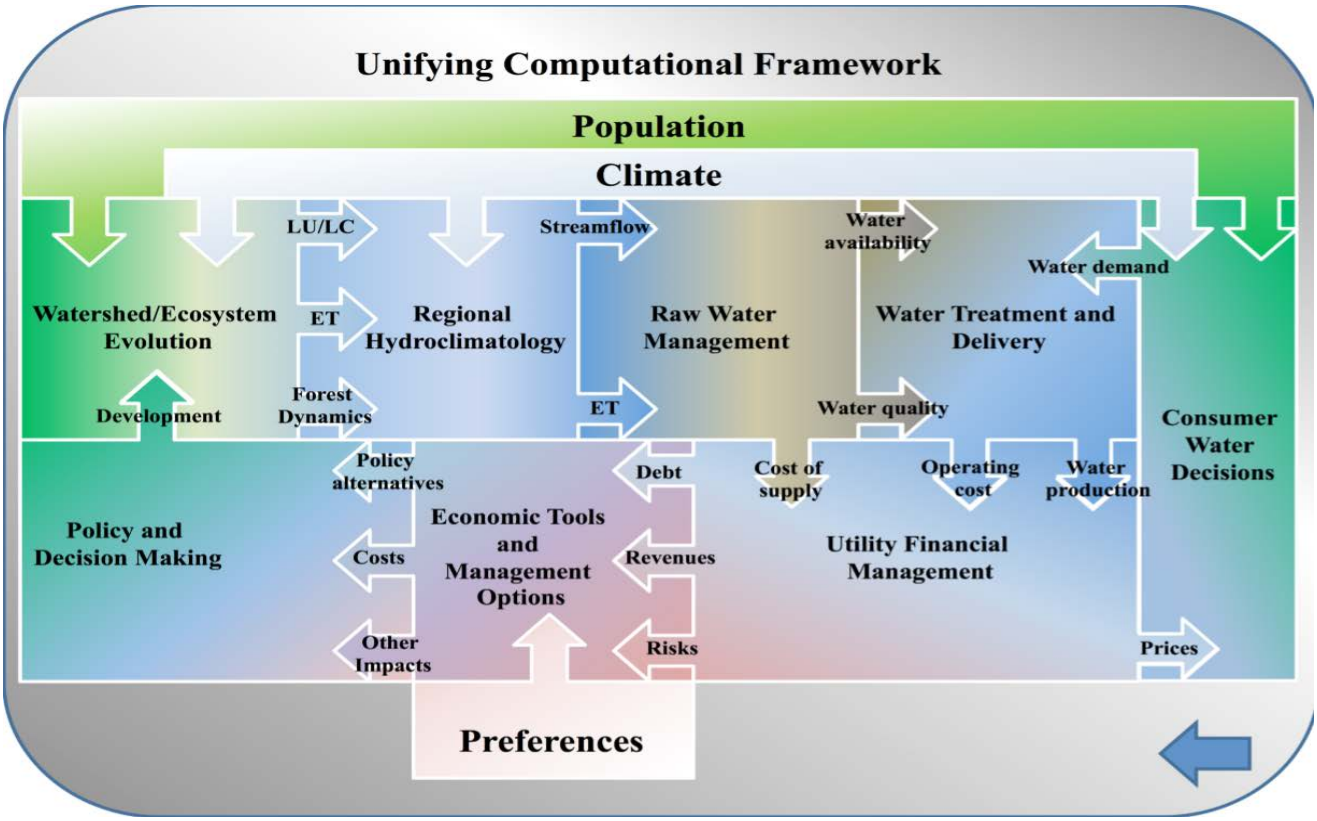

Figure 6: *Flow chart developed to evaluate perturbations on water use systems to reduce or eliminate the effect of drought.*

Improve monitoring of transport through porous systems. (3D, real-time, in-situ, ambient, multiple length scales): Central to the evaluation of INFEWS is the ability to monitor transport of nutrients, water, and energy in real-time. Identification of potential nutrient and water deficiencies in real-time and at the source will help in both the preservation of precious nutrients and the associated costs, both monetary and environmental. For example, evaluating the movement of water through soil as a function of agricultural constituents, regions, and season will greatly aid the distribution and use of precious water resources.[11] This will in turn positively affect the prevalent problem of runoff and degrading soil that is now commonly seen in the agricultural community.[11] Fundamental research to evaluate transport of water and nutrients through porous media is essential for determining the optimal irrigation and fertilizer use to reduce or eliminate waste and runoff that can re-enter the water cycle. Model systems evaluated in the laboratory will be vital to the determination of transport through complex, porous media.

Improve sample preparation and separation technologies from complex matrixes: Samples for analysis to answer INFEWS questions are often both complex and dilute, making sample preparation and analysis difficult. Analytical chemists have an opportunity to optimize sample preparation and separation technologies for the evaluation of these trace elements. The ability to concentrate these compounds will often change the outcome of the experiment and lead to errant conclusions about the content of dilute samples. Furthermore, the complexity of these mixtures necessitates the ability to finely separate compounds, some of which are unknown. As demonstrated in Figure 7, there are many potential sources and transformation products of contaminants found in both water sources and purified drinking water. The ability to define these compounds will greatly enhance the chemist's ability to determine the source and content of water contamination.

Measuring a wide range of unknown organics of soil and seawater: The complexity of INFEWS requires evaluation of mixtures, trace compounds, and unknown materials. An example is the isolation of drugs, drug products, and nanomaterials from streams.[10] Chemists isolate water from

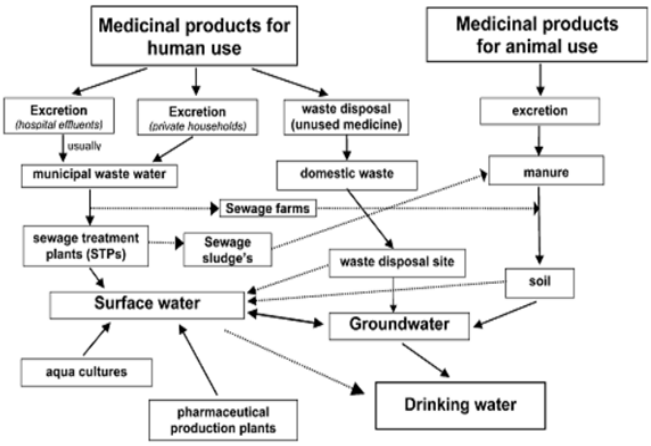

Figure 7. *Potential sources and movement of contaminants through the water cycle. Each component must be evaluated for its content and transformation product contamination.*

streams to find trace amounts of drugs, which is evaluated by careful sample preparation of a mixture of compounds. In addition, the transformation products of these drugs are largely unknown resulting from oxidation-reduction reactions, enzymatic biodegradation, and coupling reactions to other chemical species present in the environment. The evaluation of these transformation products and their presence in streams is largely unknown. Not only are these chemicals observed at extremely low levels in streams, the uncertainty of the chemical structure of transformation products presents a large challenge to the evaluation of the true environmental impact of these drugs. Furthermore, the effects of transformation products on aquatic life or the mechanisms for these drugs and transformation products interact in synergistic or detrimental ways is not understood.

Development of standards and libraries: The development of standards and libraries to aid researchers in addressing these complex mixture questions would significantly accelerate the progress in understanding how drugs and their transformation products affect aquatic life. Data sharing across the world, especially in the identification of transformation products, would provide researchers a basis for which to explore the interaction of these chemicals with each other and with aquatic life.

Low cost, real-time, multi-parametric sensors for optimizing water and nutrient use efficiency: Low-cost environmental sensors are suitable to mitigate environmental health throughout the INFEWS community.

Similar to strategies used in the biomedical community, the development of zero-energy, cost effective devices is necessary to translate findings in the lab to the INFEWS user. The development of low-cost sensors to evaluate water quality at the source will greatly aid in the evaluation of how drugs and their transformation products move throughout the ecosystem to affect water quality and aquatic life. Low-cost sensors to assess plant health, soil properties, and water quality would provide farmers a quantitative metric with which to evaluate the health of their fields and crops. This would greatly reduce the amount of fertilizer and water necessary to sustain crops, as those resources would only be used when the plant is in need.

VIII. Macromolecular and Supramolecular Chemistry across Length Scales with Bio-inspiration

Providing sustainable supplies of purified water, energy, and food is a critical global challenge for the future. INFEWS are inherently linked since clean water is required to produce food and energy, and energy is required to purify water and produce food. As populations continue to grow, society will rely more heavily on purified water from increasingly saline and contaminated sources, alternative and emerging clean energy technologies, and innovative food production strategies. In addition, an increase in industrial development requires substantial expansions of both energy and purified water resources. For example, if future energy demand is met using thermoelectric power plants, an additional 2.6 billion gallons of cost-effective supplies of clean water are required per day by 2030 (a ~40% increase of water and energy using energy efficient and environmentally friendly technologies).

The polymer chemistry of membranes will play a key role in addressing these clear and pressing global needs for water and energy. Membranes are widely used in desalination applications, such as reverse osmosis (RO), nanofiltration (NF), forward osmosis (FO), membrane assisted capacitive de-ionization (MCDI), and electrodialysis (ED), and they could be critical for emerging power generation and storage technologies including pressure-retarded osmosis (PRO), capacitive mixing (CAPMIX), reverse electrodialysis (RED), and aqueous and non-aqueous batteries. All of these technologies rely, at least to some extent, on membranes to control rates of water and/or ion transport.

The worldwide demand for new sources of water is growing exponentially, driven by rising population and rising climate variability. Novel materials offer great promise for the improvement of systems for water treatment, wastewater reuse, and desalination. Materials that inhibit biofilms, resist chlorine, separate organics, limit scale formation, or in particular, materials that lead to more permeable membranes, have all been developed recently. Some of these innovations may lead to greater energy efficiency, longer maintenance cycles, simplified pretreatment, and lower overall cost of water; but others will fall short of initial expectations on one or more essential metrics. Careful scientific analysis, and system level engineering assessments, should precede the formation of start-ups and venture investment.

Interesting recent developments include graphene desalination membranes and grafted iCVD coatings that resist bacterial adhesion and tolerate chlorine. Polymer reverse osmosis membranes must achieve target flux at slightly lower applied pressure with high salt rejection. Various nanoporous membranes with reports of very high permeability, engineered surfaces that differentially control contact angles for water and oil, and forward osmosis claim low-energy draw regeneration and additives that precipitate dissolved salts.

While creative thinking is the key to all forward progress, some early stage reports have fallen into unfounded proposals, with the equivalent of perpetual motion machines being proposed, funded, and even commercialized. Yet, simple thermodynamic assessments set an unavoidable baseline for the ultimate energetic performance of a system embedding any particular material. The separation of pure water from an aqueous solution at infinitesimal recovery, requires a minimum molar energy $\Delta G = -RT \ln a_w$; and most desalination systems operate at finite water recovery, with a higher minimum energy requirement. Further, the activity of water, a_w, rises substantially in moving from brackish groundwater, to seawater, to wastewater from oil/gas extraction. The calculations are classical, although in most cases, precise results require a mixed electrolyte model, such as Pitzer-Kim. Today's best systems are within a factor of two of the thermodynamic minimum. However, claims of energy reduction by orders-of-magnitude are common.

The world is in critical need of better solutions for water supply, and all of our creativity and insight should be applied to finding these solutions. However, we must remember that evaluations of constraints earlier in the innovation cycle will speed our overall progress.

Grand Challenge 6: Design and characterization of macro-molecular and supramolecular materials to improve water efficiency/quality and food production

Water purification membranes require understanding fouling, scaling, and lifetime prediction: Current RO membranes are fabricated from polyamide polymers. A common disinfectant used for preventing fouling is chlorine; however, polyamide is not stable to chlorine exposure. There is a need for chlorine stable membranes. Similarly, in residential applications, scaling due to $CaCO_3$ is a major issue. Designing membranes with surfaces resistant to scale formation will be impactful.

The next generation of water purification membranes will implement bio-inspiration through the generation of aquaporins into synthetic membranes. Aquaporins naturally filter pure water into and out of cells to maintain a constant osmotic pressure. The utilization of these pores in a rational, cost-effective way will provide membranes with natural selectivity for water. In addition, the incorporation of these aquaporins has the potential to eliminate many of the issues surrounding water purification, including chlorine sensitivities and fouling.

Develop structure-property-performance relationships using rational design and materials genomics for membranes: Much remains unknown about the influence of polymer chemistry, structure/morphology, and processing conditions on fundamental water and ion transport properties. Understanding ion-polymer interactions and chemistry at the molecular level will catalyze preparation of desalination membranes that achieve favorable combinations of high water permeability and high salt rejection to overcome the commonly observed tradeoff relationship where highly water permeable polymers tend to have low water/salt selectivity and *vice versa*. Additionally, fundamental understanding of relationships between polymer structure and ion-polymer interactions will enable preparation of improved membrane polymers for electric potential field-driven applications where exclusion of certain ions from polymers is critical for preparing highly efficient permselective membranes with low ionic resistance. Finally, understanding the influence of chemistry and processing conditions on polymer morphology and properties will be critical for developing high performance membranes. Preparation of next generation polymer membranes will rely on new chemistries guided by fundamental structure-property-processing relationships. Such materials will be critical for enabling new and innovative technologies to address FEWS nexus challenges.

Ionic interactions with chemical structure and morphology: Whether in agriculture, water purification, or energy movement and storage, the interactions between ions and their surroundings plays a large role at INFEWS interfaces. In water purification, the concentration and content of these ions will greatly influence the ability of a membrane to foul or remain pristine. The ion content in soils can change how water is absorbed and how plants can uptake nutrients. The concentration and types of these ions can then affect crop health and crop yields. The movement of ions and the efficient storage of these ions has long been the concern of scientists pursuing sustainable energy. Fundamental studies to evaluate how these ions interact with their surroundings, both in model systems and mathematical modeling is essential to determining how these ions can affect INFEWS.

Materials to improve food quality and safety (shelf life): Food borne illnesses are a major issue within the food supply. Once an outbreak is suspected, the response is often to remove all potential contaminated food and destroy it. This results in a loss of both food and revenue. The development of "smart" packaging that can protect food from pathogens and other detrimental contaminants, monitor food quality such that suppliers can identify compromised products and remove them, and report information to suppliers to assist in tracking the source of the problem.

Bio-inspired structure for energy storage, energy generation, water management, and water filtration: Biological entities have evolved to efficiently store and generate energy, as shown in Figure 8. In addition, the complexity of soil and vegetation that naturally purifies water offers a natural solution to the generation of clean water. Further understanding of these systems, their composition, and movement of energy and water through them is essential for the next generation of INFEWS solutions. For example, the generation of synthetic aquaporins for use as water purification membranes has long been an attractive avenue for extremely efficient water purification. The evaluation of these biologic systems and the determination of how their natural processes are useful for INFEWS solutions are vital to solving these grand challenges.

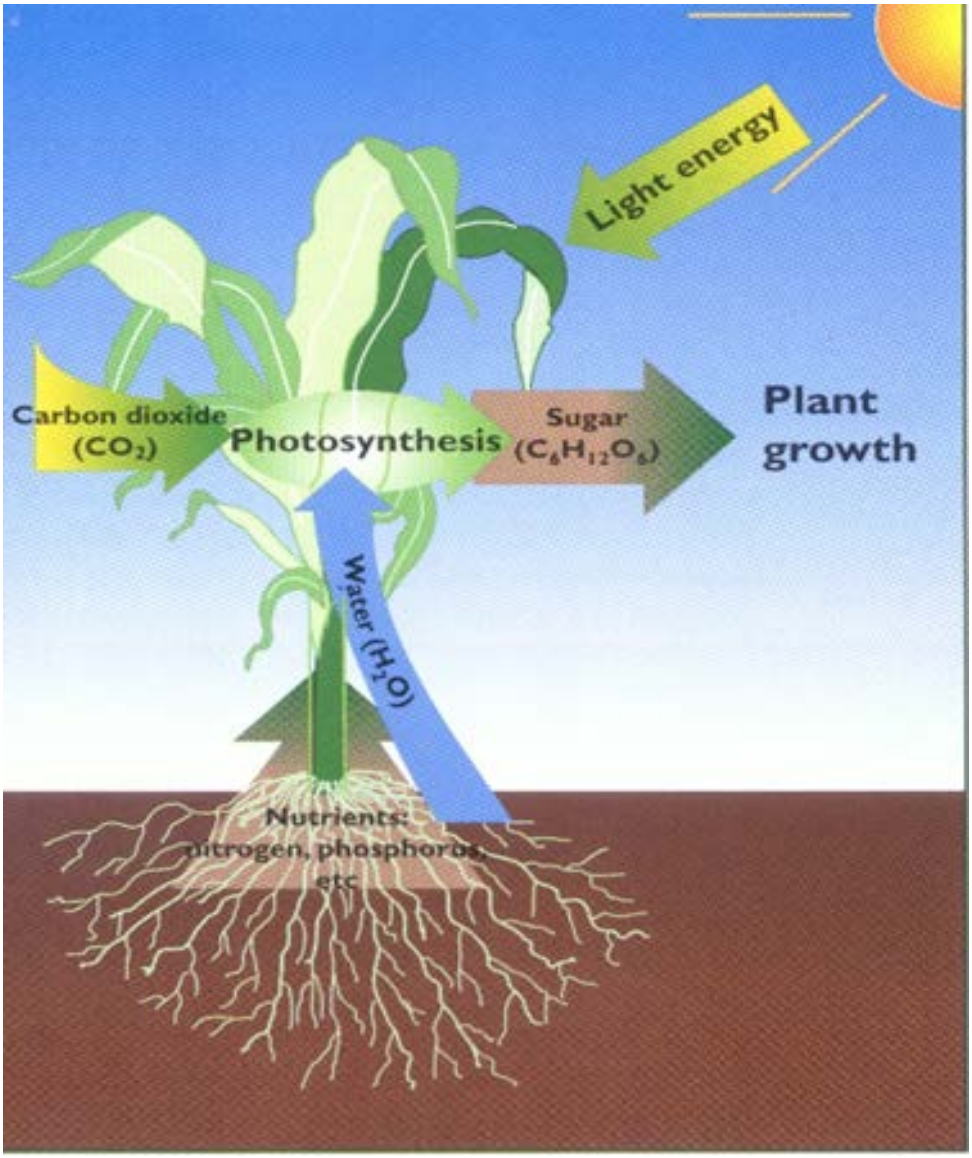

Figure 8: *Inspiration for bio-mimicking energy production and storage. Natural water purification also depends on soil and plant health*

IX. Understanding Surface Phenomena at the Biology-Chemistry Interface

Surfaces dominate the transport and availability of nutrients in INFEWS. From the surface of membranes used to purify water to the interaction between air, water, and soil in the irrigation of agricultural fields, surfaces and surface interactions play a large role. Understanding these complex surfaces, their interactions with substituents, and their dynamic changes over time is essential to solving many INFEWS issues currently plaguing our environment.

Grand Challenge 7: Revealing surface chemistry and interfacial phenomena important to the INFEWS nexus

Understanding the nanoscience of bio-systems and implications on purification systems: One of the most important surfaces for INFEWS is that of water purification membranes. The evaluation of how bacteria and other biological entities adsorb and bind to water purification membranes to cause fouling is largely unknown. The fundamental evaluation of biological systems and the mechanism of absorption onto these complex surfaces are essential to the evaluation of biofouling. The answers to these fundamental questions can then drive the development of new water purification membranes that can prevent this biofouling, which in turn will reduce the cost and energy required, as well as increase the lifetime of these membranes.

Elucidating specific and nonspecific interactions on surfaces (metal and nutrient adsorption): Evaluating metal and nutrient adsorption to surfaces is essential to predict soil health, plant health, and in turn the water adsorption properties of that soil. Whether these interactions are specific, such as specific nutrient adsorption by the microbiota found in soil, or non-specific, is a question vital for the development of solutions to INFEWS issues. How these metals and nutrients adsorb into the soil surface can then drive the introduction of fertilizers and nutrients to the system. Determining the concentration and content of these moieties on the soil surface is essential to determine the optimal fertilizer and irrigation schedule. The initial interaction of these moieties with the soil surface is the first step to answering these questions.

Chemical topology at surfaces in concert with intermolecular interactions: Chemical topology is essential to understand how molecules interact with surfaces. Surface roughness, wettability, and chemical structure play a large role in how water and nutrients will adsorb onto these surfaces. For example, water purification membranes often have defects and a surface roughness at a small scale; the evaluation of these defects on how water and fouling moieties adsorb onto the surface can drive rapid improvements to water purification membranes. Topology, however, is not the only answer to this surface issue. Intermolecular interactions, whether electrostatic or a concert of hydrogen bonds, will also play a large role in the interactions between solutes and the surface. The chemical structure of water purification and energy membranes is essential for solute interaction, whether favorable or unfavorable. The concert of chemical structure and topology will drive the interactions between membranes and solutes. Structure-property relationships

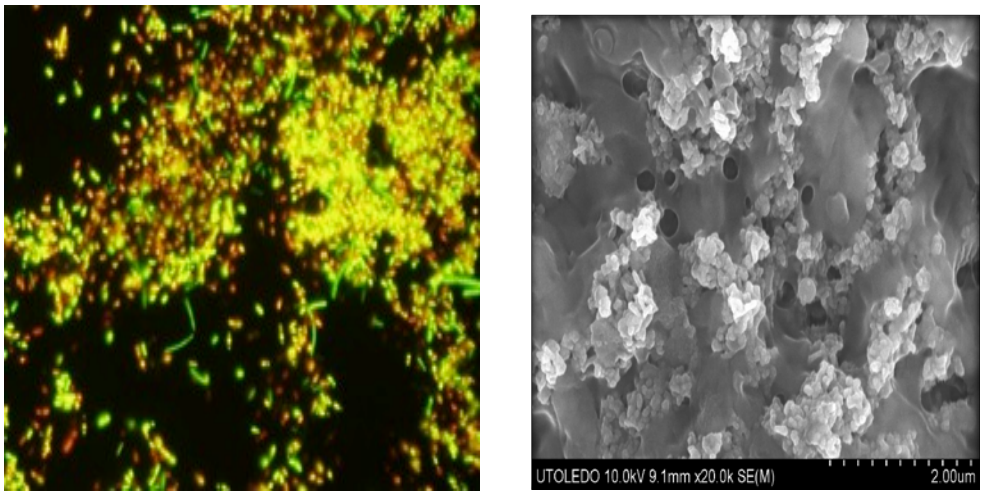

Figure 9: *Cells detached from a biofouled membrane, stained with either PI or pico-green and imaged using a fluorescent microscope (left), and imaged using scanning electron microscopy (right)* [1].

and a variety of solutes are essential for the fundamental understanding of these interactions.

Mechanistic understanding of biofilm formation in membranes and soil: Biofouling is the accumulation and growth of microorganisms onto the membrane surface, as shown in Figure 9. Biofouling of membrane surfaces occurs in a few general phases. Initially, the surface to which the biofilm attaches will become conditioned with a range of organic molecules that rapidly adsorb to the surface upon exposure to an aqueous environment. These molecules include proteins, polysaccharides, nucleic acids, humic acids, lipids, fatty acids, pollutants, etc.[12] Then, primary colonization occurs where adhesion is essentially proportional to the cell density in the water phase and occurs owing to weak physicochemical interactions. It is thought that the microorganisms that initially attach during this phase are often in starvation/survival phase and tend to be smaller in size and secreting a higher ratio of extra cellular polysaccharides.[12] It has been shown that higher amounts of extracellular polymeric substances are directly related to cellular adhesion.[13] This primary colonization is then followed by the logarithmical growth phase, when cell growth on the surface contributes more to biofilm accumulation than does the adhesion of planktonic cells. Essentially, the cells which have attached to the conditioned surface can now feed off the nutrients which are concentrated at the membrane surface, due to rejection by the membrane's selective layer, and multiply.[14] Finally, a plateau phase, when biofilm growth (adhesion and cell multiplication) and cell detachment are in balance, occurs. This phase is controlled by the nutrient concentration and the resultant growth rate, the mechanical stability of the biofilm, and the effective shear forces. In addition, it is independent of the concentration of cells in the raw water. It is also thought that during this stage subsequent production of extracellular polymers occurs.[15] Improving the fundamental understanding of microbial adhesion to surfaces can provide crosscutting innovations in INFEW systems.

Biofouling can cause a flux decline by two methods: (i) an increase of the hydraulic resistance over the membrane and (ii) hindering the back diffusion of salts.[16] Biofouling is especially problematic because biofilms occurring in membrane systems may cause severe loss of performance and the use of costly cleaning procedures to maintain output and quality. Frequently, the fouling can be so severe that operation cannot be maintained and membrane replacement is needed.[17]

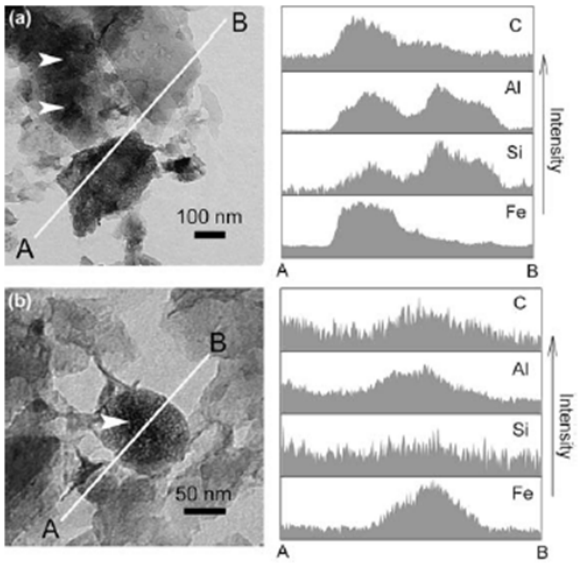

Figure 10*: TEM images and cross-section elemental analysis of clay fractions (<2 μm) from two subsurface soils. Organo-mineral associations in the colloidal size range (< 2μm) form the basic building blocks of soil structure.*

Wetting on heterogeneous dynamic surfaces: Water adsorption on soil surfaces is affected by erosion and years of agricultural use; topsoil degradation and erosion cannot be fixed easily by nature, as soil formation takes thousands of years. The chemistry of the topsoil changes as a function of all these factors, which in turn changes the wettability and intermolecular forces acting on the surface of the soil. Soil health is also a large factor in nutrient adsorption, which is essential for plant and crop health. Chemists have a large challenge to determine what causes soil to begin to repel water (causing runoff effects in fields) and how factors such as irrigation, water composition, extracellular polymeric substances, microbiota, and nano-scale topographic changes affect the health of the soil. Development of a relevant artificial soil to study these phenomena as well as provide a viable option for topsoil replacement is necessary to address these challenges in the agricultural community. A complex evaluation of the microbiota composition in the soil is needed to evaluate how these species interact with each other and their environment; how these microbiota change as the soil changes with irrigation is also necessary to determine any relation to water repellency. Furthermore, the evaluation of the extracellular polymeric substances in the soil, how they change over time, and their role on water infiltration is needed to fully evaluate and provide a prediction metric for soil health over time.

X. Reactions and Separations of Complex Mixtures

Probably the most significant "Grand Challenge" for fundamental chemistry in soil research is associated with the phenomenon of soil degradation. Soil degradation is an increasing issue globally, exacerbated by climate change and affecting food security, threatening water resources and ultimately acting as a driver to migration.

Food insecurity will be exacerbated by a population increase to an estimated 9.5 billion people in 2050. As a result, crop production must outpace human population growth significantly during the next 40 years. For reasons detailed by Sposito (2013), this large relative increase in food crop production will have to come mainly from increasing crop yield per hectare planted – crop intensification – not from converting more land to agricultural use. Adding to the challenge is an increasing scarcity of "blue water", i.e. the water that is extensively withdrawn from streams, lakes and aquifers for use in irrigated agriculture. In short, more people will have to be fed based on roughly the same land area and the same amount of water as we have available today. However, the suitability of soil for agriculture is degrading at an alarming pace. This can be illustrated using some numbers from a recent report issued by the Economics of Land Degradation Initiative (ELD-Initiative, 2015). According to this report, 52 % of agricultural land worldwide is moderately or severely affected by soil degradation. 12 million hectares of soil are lost each year from desertification and drought alone. 44% of global food production takes place in the world's degrading drylands. Yet soils are aqueous systems, they cannot provide the ecosystem services needed by an exponentially growing global population in the absence of water. To illustrate the close relationship between soil, water and energy, this report defines soil and provide a brief description of this natural body. The report employs an example from irrigation agriculture in eastern Oregon to show how intensive land use can induce water repellency in soil. Current theories to explain soil water repellency will be introduced and the close mechanistic relationships between the surface chemistry of mineral and organic soil constituents and the ability of these soil constituents to aggregate into three-dimensional structures with variable porosity demonstrated. Unknowns will be identified and a role for fundamental chemistry to contribute to a better understanding of the system will be suggested.

Grand Challenge 8: Understanding chemical processes in complex mixtures

Reactions and catalysis in porous media (soil): Chemical reactions performed in the laboratory are often well defined with concentration, solvent, temperature, and mixing. However, reactions of INFEWS are often performed in complex media surrounded by void space, water, and microbiota. These chemical reactions are essential to soil health, nutrient delivery, and water transport, but are largely not understood. How the chemical reactions are influenced by soil composition and the presence of void spaces will aid in the determination of both soil health and nutrient fate. Evaluation of these reactions in controlled environments to isolate the influence of one factor is an essential part to this challenge.

Metal and nutrient chemistry and fate in soil and water: The overall determinant of acceptable water quality for food/agriculture, energy use, and drinking is based on its total dissolved solids (TDS) which are also known as “salinity” (Table 1). TDS is an aggregate measure of the amount of anions and cations in water; TDS can be highly variable for fresh water and drinking water. For example, drinking water in the 100 largest cities in the United States, ranged from 22 - 1,589 mg/L TDS with a median of 186 mg/L TDS.[18] Those at the upper range exceed USEPA organoleptic guidelines for drinking water.

Concentrations of individual anions and cations vary greatly among waters and further influence the suitability of water for a given use. Fresh waters in contact with limestone lithography typically contain calcium and carbonates, while those in contact with gypsum contain calcium and sulfate. For human consumption, consumers may detect an unacceptable salty taste in water when the sulfate concentration exceed 250 mg/L[19] or the sodium concentration exceeds the range of 30 to 60 mg Na/L.[20,21] Corrosion and scaling of metal pipes (e.g., iron, copper, lead) and polymer membranes and pipes are affected by the relative amounts of bicarbonate, calcium, carbonate, chloride, sodium and sulfate in water.[22,23] Corrosion and scaling are widely acknowledged to interfere with energy production both by interfering with heat transfer and increasing pipe roughness and therefore the cost of pumping water. Dairy cows, which typically consume 20-30 gallons of water per day, are very susceptible to diarrhea

when the sulfate concentration exceeds < 1000 mg/L SO_4^{2-} and fatality can occur when nitrate concentrations are in the range of 177-443 mg/L NO_3^-.[24] Crops are particularly susceptible to sodium and chloride, which can be detrimental to plant health and food production when too high.[25]

Water Type	TDS, mg/L
Human Drinking Water EPA organoleptic guideline (1) Situationally acceptable (2,3)	 < 500 ~ 1,000
Freshwater	0 to ~ 5,000
Brackish Water	5,000 - 30,000
Saline water	30,000 - 50,000
Brine	> 50,000
Hydraulic fracturing water (4,5,6)	250,000 - 460,000

Table 1: *Total dissolved solids in common sources of water.*

Resource recycling (ex. brine management, nutrients): The development of strategies for the recovery of nutrients and energy from urban and industrial wastewater required an integrated approach to not only identify effective and economical extraction processes, but also markets and allocation to these materials and energy. Develop and implement emerging wastewater treatment technologies focused on the recovery of nitrogen and phosphorous compounds, requires a cultural and technological shift in the way we design and operate these facilities. Additionally, it will require the development of new processes and material to achieve cost-effective recovery of nutrients suitable for agricultural applications, e.g., membrane-bioflocculation/anaerobic digestion/nutrient recovery. This treatment train has been proposed by few researchers as an efficient four steps treatment systems that provide high quality effluent, allows nutrient recovery and produce energy.[26-28] During the first stage, accumulation of organic matter occurs through the simultaneous membrane separation and bioflocculation by microorganisms excreting extracellular polymers (EPS) that flocculate suspended and colloidal organic matter. Bioflocculation is achieved by promoting the growth of EPS-forming microorganism using low solid retention time of 0.5–1 day,[29] very low in comparison with 30 days commonly used in conventional WWTP. The biosolid obtained in this stage contain a high organic matter concentration, which is used as influent for the second stage of the process, anaerobic digestion.[28] The anaerobic digestion process consists of a microbial consortia that can treat biosolid reducing its volume, organic and pathogenic content and produce methane. Finally in a third stage, the liquid resulting from the bioflocculation will be treated in two steps first cold partial nitration and Anammox followed by phosphorus recovery process. In the partial nitritation stage, ammonium is partly nitrified to nitrite.[30,31] In the Anammox stage, the produced nitrite is biologically denitrified in combination with the residual ammonium to nitrogen gas and nitrate.[27,32] This process requires lower energy consumption for aeration in comparison to conventional nitrification/denitrification process, as only part of the ammonium is nitrified. Additionally, this process does not require the addition of external carbon source due to the Anammox autotrophic denitrification characteristics. Laboratory and pilot scale studies have shown that the partial nitritation/Anammox could be operated at low sewage temperatures between 10 and 20 °C and dilute N sewage concentrations (<100 mg N/L).[33] Finally after the nitrogen removal treatment, phosphorus recovery will take place at low temperature using processes such as reversible adsorption of phosphates on iron oxides.[34]

Supramolecular interactions in aqueous systems: Key constituents of soil and water systems, e.g., natural organic matter matrices, are relatively unknown in terms of chemical composition. Addition of anthropogenic compounds and biogeochemical transformations of these makes the soup of potential reactants even more complex. The first challenge is to identify the key reactants in soil and water that cause significant biological and toxicological impact. At what concentrations and mixtures do these chemical components provide impact? How do we address non-linear synergies in the reactions and biological responses? Because these systems are so intertwined, we need to pull them into tractable fractions for further analyses and controlled reactions. The challenge, upon addressing this analytical goal, will be developing appropriate statistical approaches and predictive chemical and coupled physical-chemical models. This approach will allow for reassembling these tractable pieces into environmentally relevant wholes.

XI. Targeted Delivery for Sustainability at the FEWS Intersection

Non-specific interactions between nutrients, water, vegetation, and synthetic membranes can cause a large range of problems that affect the sustainability of INFEWS. To more effectively deliver nutrients and eliminate potential sources of contamination downstream, there is a great need for targeted delivery systems. This includes the targeted delivery of water directly to plants when they need it, as well as the targeted delivery of fertilizers. The elimination of waste nutrients from the water and food cycle will aid largely in the elimination of contaminated water, degraded soil, and excess use of energy.

Grand Challenge 9: Protecting water resources by targeting the delivery and understanding the fate and transport of bioactive compounds

Compiling data sets to determine causation and understanding synergistic toxicological effects: The dissemination of data across disciplines to evaluate the potential causes of water contamination and toxicological effects is essential to answer these grand questions in water chemistry. As an example, pharmacological chemists that evaluate potential drug transformation products as a result of oxidation, reduction, or chemical reactions have a duty to share this information with scientists evaluating the quality of water found in streams contaminated with drugs and their transformation products. As these compounds are evaluated and identified, potential toxicity concerns to aquatic life can be more accurately assessed. The effective elimination of these compounds from wastewater before they enter aquatic environments is an attractive solution to prevent errant toxicity to aquatic life.

Develop mechanisms to selectively deliver pest management chemicals (molecular recognition, encapsulants, pro-compounds, biodegradability) to targets to protect water resources and the end user: Agriculture relies heavily on effective delivery of agrochemicals to provide nutrients, aid in crop/animal protection, and regulate commodity growth/development at specific times in the production cycle. Yet many agrochemical delivery technologies are decades old and fail to benefit from recent advances in chemistry/engineering that enable other industries to precisely deliver chemicals to a target (i.e. pharmaceuticals).This research could benefit all agricultural sectors, as well as society as a whole, by serving as a catalyst for engineering and field-testing of a new generation of improved agrochemicals with superior efficacy/efficiency/ longevity/safety and hence enhanced environmental and economic sustainability. By combining persons of diverse, transdisciplinary backgrounds, we hope this grand challenge serves as the catalyst for multiple proposals that will be submitted to NSF, USDA-NIFA (or similar) funding agencies, fostering innovation across many agricultural systems over the next decade or longer. We also hope to serve as the genesis of lasting private/public R&D partnerships.

In the last several years, there has been increasing emphasis on basic science that addresses potential agrochemical delivery systems.[35-38] However; to date, no studies have adequately addressed how to translate the findings from basic science (laboratory-studies) to industry-level application. Specifically, can novel delivery systems produced in the lab be translated to the manufacturing, delivery (shipping) and application (farm) processes? That is the goal of this grand challenge, and it can only be successfully addressed if persons from laboratory, manufacturing, distribution and application niches combine forces. In addition, efforts should be made to identify additional stakeholders and expertise that can inform the strategic plan and resulting proposals to private and government agencies.

“Controlled-release” (polymer-coated or impregnated) fertilizers are an example of an agrochemical delivery system that, while strides have been made to increase efficiency, could possibly benefit from newer technologies. Studies have shown that a significant portion of mineral nutrients are released in the first 25-33% of the labeled release period, resulting in a failure to provide labeled longevity. Today, controlled release fertilizers (CRFs) are unreliable, prone to variation due to weather and soil chemistry. Inefficiency of CRFs reduces cost-effectiveness and results in nutrient leaching. Leaching in turn contributes to non-point source runoff and degradation of impaired waterways that provide drinking water to millions of citizen-stakeholders. This example illustrates the need for a new generation of agrochemical carriers that enhance the longevity, efficiency, and efficacy of agrochemicals

and the crosscutting benefit from producer to environment to society. This philosophy mitigates the problem from the input-side rather than the output-side of the production cycle, in theory increasing efficiency of the applied agrochemical and therefore also improving profitability.

Related ongoing or recently completed significant activities related to this project: There has been a continuous effort over the past four to five decades to improve agrochemical use efficiency. Much of this work has occurred with nutrient use efficiency.[39-44] The use of CRFs allow growers to increase nutrient use efficiency (NUE; namely nitrogen and phosphorus) by supplying mineral nutrients corresponding with plant demand and minimize pathways or processes of losses (microbial transformation, soil fixation, leaching), thus decreasing environmental impact.[45] Despite this, nutrient use efficiency remains low in most cropping systems. Chemistries that would be useful in the controlled application of agrochemicals include encapsulation technologies, polymer systems, stimuli-induced materials, and other material science innovations that can improve control and targeted release. Advanced materials coupled with improved application technologies, could maximize crop mineral nutrient use and minimize environmental impact.

XII. Acknowledgements

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XIII. Appendices

Appendix A - Workshop Schedule

Tuesday, October 13, 2015 (NSF)

5:00 PM to 7:00 PM	**Registration and Welcoming Reception** (Opening Remarks, Workshop Co-Organizers)

Wednesday, October 14, 2015 (NSF)

Invited lecture durations are set at 40 min (30 min lecture with 10 min for Q/A), although this time may be reduced to increase break-out session lengths. All general lectures will be held in the E/W Falls Church Room.

The breakout sessions have been broken into 6 groups of 6. Locations for each group are: Group #1 - McPherson Square Room; Group #2 - Smithsonian Room; Group #3 - Farragut West Room; Groups #4, #5, & #6 will meet in the E/W Falls Church Room.

7:30 AM to 8:30 AM	**Registration** *(registration desk will remain open until 9:30am)*
8:00 AM to 8:20 AM	**Continental Breakfast** (E/W Falls Church Room)
8:20 AM to 8:30 AM	**Welcome Remarks** - Dr. Carol Bessel *(Division Director of Division of Chemistry, NSF) and Dr. JoAnn Lighty (Division Director of Division of Chemical, Bioengineering, Environmental, & Transport Systems (CBET) (E/W Falls Church Room)*
8:30 AM to 9:10 AM	**Lecture 1: Dr. Abhishek Roy, Dow Chemical** "FEW Innovations Resulting from Fundamental Chemistry: An Industrial Perspective"
9:10 AM to 9:50 AM	**Lecture 2: Dr. Lucy M. Camacho, Texas A&M University-Kingsville** "Understanding the Intersection on Energy and Water Utilization and Infrastrcture"
9:50 AM to 10:30 AM	**Lecture 3: Dr. Markus Kleber, Oregon State** "The Intersection of Soil Science and Food Production with the Water-Energy Nexus"
10:30 AM to 10:40 AM	**Break**
10:40 AM to 11:10 AM	**Panel Discussion** *(Lecturers)*
11:10 AM to 11:50 AM	**Lecture 4: Dr. Jay Lund, University of California, Davis** "Hurdles to Water Efficiency and Alternate Supply in Agriculture"
11:50 AM to 12:45 PM	**Working Lunch**
12:45 PM to 1:00 PM	**Review of Guidelines for Break-Out Sessions**
1:00 PM to 2:00 PM	**Break-Out Session 1** - *(Opportunities for Fundamental Chemistry to Address Grand Challenges; 6 interdisciplinary participants for each break-out group)*
2:00 PM to 2:30 PM	**Reports from Break-Out Sessions** *(Posed fundamental scientific questions) - see above for group locations*
2:30 PM to 2:45 PM	**Break**
2:45 PM to 3:25 PM	**Lecture 5: Dr. John Lienhard, MIT** "Energy Requirements of Desalination: Will New Materials Help?"
3:25 PM to 4:35 PM	**Lecture 6: Dr. Warren Dick, Ohio State-OARDC** "Crop Nutrient Life Cycle Management: Impacts on Soil and Water Quality"
4:35 PM to 5:30 PM	***Break-Out Session 2*** *(Identifying Grand Challenges for Chemistry)* *Reports from Break-Out Session 2*
6:00 PM to 7:30 PM	***Dinner*** *(as a group) - Italian Restaurant (downstairs) - set menu*

Thursday, October 15, 2015 (NSF)

8:00 AM to 8:30 AM	***Continental Breakfast*** *(E/W Falls Church Foyer)*
8:30 AM to 9:10 AM	***Lecture 7: Dr. Greg W. Characklis, Univ. of North Carolina at Chapel Hill*** *"Managing Water Scarcity: Integrating Technical, Institutional and Societal Factors"*
9:10 AM to 9:50 AM	***Lecture 8: Dr. Geoffrey M. Geise, The University of Virginia*** *"Grand Challenges for Fresh Water Availability and Emerging Polymer Membrane Technologies for Water Purification"*
9:50 AM to 10:30 AM	***Lecture 9: Dr. Susan Olesik, Ohio State*** *"Monitoring and Modeling to Ensure the Quality and Security of Water and Soils"*
10:30 AM to 10:45 AM	***Break***
10:45 AM to 11:20 AM	***Panel Discussion*** *(Lecturers)*
11:15 AM to 11:55 AM	***Lecture 10: Dr. Robert D. Allen, IBM Almaden*** *"A Three-Pronged Approach to Breakthrough Materials Innovation to Solve Grand Challenges"*
11:55 AM to 12:30 PM	***Lecture 11: Dr. Carol Bessel, NSF Chemistry Division*** *"NSF Innovations at the Nexus of Food, Energy, and Water"*
12:30 PM to 1:00 PM	***Working Lunch***
1:00 PM to 2:30 PM	***Break-Out Session 1***
2:30 PM to 2:45 PM	***Break***
2:45 PM to 3:25 PM	***Lecture 12: Dr. Karen DePauw, Graduate Life Center, Virginia Tech*** *"Workforce of the Future at the Food-Energy-Water Nexus"*
3:25 PM to 5:00 PM	***Constructing a FEWS Road-Map for the Impact of Chemistry*** *(The workshop will provide a road-map and a prospectus/report; working groups will craft sections of the report based on fundamental questions/challenges of science and engineering as generated in the working groups)*
5:00 PM to 5:30 PM	***Closing Remarks and Path Forward***
5:30 PM	***Adjourn***

Appendix B - Workshop Participants

Workshop participants included a diverse interdisciplinary group of scientists with a wide range of expertise and National Science Foundation observers.

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Appendix C - Selected References

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Appendix D – Sponsors

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Website hosted by the Macromolecules and Interfaces Institute (MII) at Virginia Tech

Appendix E – Selected PowerPoint Presentations from Participants

Copies of the slide presentations can be downloaded from the workshop website (http://www.mii.vt.edu/nsfworkshop/).