Title: Sustainable Water through Innovation in Membranes & Materials (SWIMM)

Lead Faculty: Stephen Martin (Chemical Engineering); Robert Moore (Chemistry)

Faculty Member	Department	College
Stephen Martin	Chemical Engineering	COE
Donald Baird	Chemical Engineering	COE
Luke Achenie	Chemical Engineering	COE
Sanket Deshmukh	Chemical Engineering	COE
Johan Foster	Materials Science & Engineering	COE
Jason He	Civil & Environmental Engineering	COE
Peter Vikesland	Civil & Environmental Engineering	COE
Marc Edwards	Civil & Environmental Engineering	COE
Andrea Dietrich	Civil & Environmental Engineering	COE
David Dillard	Biomedical Engineering & Mechanics	COE
Jack Lesko	Biomedical Engineering & Mechanics	COE
Robert Moore	Chemistry	COS
Tim Long	Chemistry	COS
Judy Riffle	Chemistry	COS
Amanda Morris	Chemistry	COS
Shengfeng Cheng	Physics	COS
Kevin Edgar	Sustainable Biomaterials	CNRE
Klaus Moeltner	Agricultural & Applied Economics	CALS
Kang Xia	Crop & Soil Environmental Sciences	CALS
Ryan Stewart	Crop & Soil Environmental Sciences	CALS
Brian Badgley	Crop & Soil Environmental Sciences	CALS
Valisa Hedrick	Human Nutrition, Foods, and Exercise	CALS
Julia M. Gohlke	Population Health Sciences	Vet Med
Susan Duncan	Food Science and Technology	CALS

1. Vision Statement

In 2012, the United Nations reported that water scarcity affects every continent.[1] Around 700 million people in 43 countries currently face water shortages or lack access to clean drinking water. By 2025, 1.8 billion people will be living in countries or regions with absolute water scarcity, and two-thirds of the world's population could be living under water stressed conditions. Water scarcity is mainly caused by overwhelming human consumption and contamination, from production of water-thirsty meats and vegetables, biofuel crop production, industrial uses, and rapid urbanization.[2] The scale of water scarcity makes it an interconnected global issue and efforts to minimize the gap between water supply and demand are critical. Although over 70% of the surface of the earth is covered with water, less than 1% is easily accessible fresh water. Moreover, the distribution of fresh water is not even over the globe.[3] Fresh water sources (e.g., rivers, lakes, groundwater) are increasingly being degraded below a usable quality for agriculture, industry, and drinking from anthropogenic inputs of inorganic (Anning and Flynn, 2012) and organic (Koplin et al 2002) contaminants. The generation and distribution of freshwater from non-potable fresh and saline sources has direct linkages to regional stability and global economic development.

Materials have an important role to play in water production, water reuse, and wastewater treatment, particularly for water purification via filtration, membrane separations, and advanced techniques such as electrodialysis. For example, total global desalination capacity has grown rapidly over the last decade and was projected to be over 100 million cubic meters (m^3) per day in 2016. This capacity is two-fold higher than global water production by desalination in 2008.[5–7] Properly designed and implemented membrane processes can be energy efficient and easily scalable, thus making them an ideal replacement for more energy intensive processes such as multi-effect distillation. Significant materials challenges still remain to the production of economical membranes with high flux, high selectivity, and good chemical and physical stability. In addition, the specific requirements vary based on the source water (i.e., sea water, brackish water, wastewater, hydraulic fracturing water, degraded fresh water) and the application (i.e., drinking water, industrial cooling water, agricultural and irrigation water, and water for food production.) This demands a multidisciplinary approach wherein application area experts work closely with researchers synthesizing new materials and fabricating novel membranes.

2. Relevance

Virginia Tech is uniquely positioned for prominence in the development and application of materials for water purification and processing due to our internationally acknowledged strengths in polymer science and engineering (MII, Chemistry, Chemical Engineering, Materials Science and Engineering), water quality and treatment (Civil and Environmental Engineering, Water Interface IGEP, Crop & Soil Environmental Sciences, Biological Systems Engineering), and sustainability (Sustainable Nanotechnology IGEP, Sustainable Biomaterials, Green Engineering). For this effort we bring together the broad expertise of a diverse group of researchers, many of whom are well-known on the national and international stages. The research team is composed of faculty spread across a number of departments and colleges, and many are already involved in ongoing research collaborations and in current interdisciplinary initiatives. The team includes faculty from the colleges of Engineering, Science, Natural Resources & the Environment, and Agriculture & Life Sciences, and departments including those identified above as well as Physics, Materials Science & Engineering,, Biomedical Engineering & Mechanics, Human Nutrition, Foods, & Exercise, and Agricultural & Applied Economics.

The goal of this program is to approach materials research for water applications for the broad range of water users and consumers. The breadth of the research team provides the capacity to link together research from diverse disciplines and over multiple scales from experimental and computational to molecular design of new materials through device fabrication, scale-up and manufacturing, process and system level modeling, and economic, environmental, and health impact and life-cycle analysis.

Relevance to GSS, the Materials SGA, and other Destination Areas: SWIMM is directly aligned with the "abundance and quality of fresh water" critical problem area identified in the GSS destination area. In addition, SWIMM is aligned with the "Environment" research pillar in the nascent Materials

SGA, and has been selected as one of 5 core research thrusts for further development. SWIMM will contribute to both the research and teaching goals of the GSS destination area. The group will leverage existing expertise, facilities, and collaborations to develop a broad, interdisciplinary research initiative in the development of new materials, devices, and systems in the critical area of sustainable water production and processing.

The proposed research area is complementary to three current Destination Areas: Intelligent Infrastructure for Human Centered Communities (IIHCC), Global System Science (GSS), Data Analytics & Decision Sciences. We envision potential interactions with IIHCC through their efforts in Smart Design and Construction, as water purification, delivery, and wastewater treatment are key elements in this area. The quantification of impacts of water production, quality, and distribution requires the analysis of large data sets, so there is clear potential for interactions with DADS.

Opportunities for Extramural Funding: Interest in water purification cuts across multiple funding sources, including government agencies and industrial sponsors. NSF has recently instituted a program for Innovations at the Nexus of Food, Energy and Water Systems (INFEWS) and this is a natural fit for the SWIMM effort. NSF has also funded Engineering Research Centers in the water area, such as the ERC on Nanofiltration at Rice University. Our approach is distinct in that we are focused on membrane-based technologies for reverse osmosis, forward osmosis, and electrodialysis applications. The USDA has recently announced an Agriculture and Food Research Initiative (AFRI) RFP in the "Water for Food Production Systems Challenge Area", which is a natural fit for the program. In addition, there are several programs at the DOE and DOE that can be targeted. Current interdisciplinary funding in these areas at Virginia Tech include the REU program in research at the Food-Energy-Water Nexus run by the Macromolecules Innovation Institute, and the NSF REU and RET programs in Water Science. With some investment, Virginia Tech will be well positioned to apply for a Center level grant (ERC or MRSEC) in the area of membrane-based water purification within the next 3-5 years.

3. Curriculum Opportunities

The SWIMM focus lends itself well to the development of interdisciplinary curricular programs in sustainable water production – efforts that tie in directly to ongoing initiatives such as Pathways to Knowledge, and the VT-shaped student concept of undergraduate education. Such an effort could include the development of a Pathways minor that ties together the social, economic, scientific, and policy issues associated with the production of potable water and the treatment of wastewater. In addition, faculty in SWIMM would take a lead role in the development of an interdisciplinary curriculum at both the undergraduate level aimed at providing students with the tools and knowledge necessary to tackle both the technical and non-technical issues associated with water production and treatment.

4. Resource Needs

Current Resources to be Leveraged for SWIMM:

- ***Experimental Facilities and Expertise:***
  - Materials Synthesis: Laboratory facilities for new materials synthesis are available in CHE, Chemistry, Sustainable Biomaterials, and CEE.
  - Materials Characterization: Extensive capabilities for materials analysis and testing are available in CHE, Chem, CEE, and BEAM. In addition, the Nanoscale Characterization and Fabrication Laboratory (NCFL - ICTAS), the NSF sponsored NanoEarth Center, and the Macromolecular Materials Discover Center (MMDC - MII) provide state of the art characterization facilities accessible to users from around the university.
  - Membrane fabrication: Fabrication facilities for lab-scale membrane production are available in CHE, Chemistry, and CEE.
  - Membrane Testing: Equipment for testing of lab-scale membranes (i.e., membrane permeation and selectivity) is available in CHE, CEE, and Chemistry.
  - Water purification system testing: Equipment for evaluating small-commercial scale membranes in water purification systems are available in CEE.

- Water quality analysis: The Environmental Organic Chemical Analysis Service Center at CSES has state-of-the-art UPLC/tandem mass spectrometry, GC/tandem mass spectrometry, molecular microbiology lab for analyzing microbial indicators and microbiomes, and other essential equipments for water testing of for analyzing organic and microbial contaminants. CEE has a state-of-the-art environmental and water resources laboratory and analytical instrumentation for detection of inorganic and organic water and air quality parameters at part per trillion concentrations and above.

- ***Modeling and Analysis:***
  - Significant expertise and capacity in molecular scale modeling (e.g., DFT, MD, CGMD), multi-scale modeling, optimization based approaches to inverse modeling, materials design and optimization, and process modeling exists in CHE and Physics.
  - Economic Modeling and Analysis expertise is drawn primarily from Agricultural and Applied Economics.
- ***Social and Environmental Impact:***
  - VT has a strong track record in tying technology issues to relevant societal and environmental needs. We have identified faculty in various departments (e.g., CEE, Crop & Soil Environmental Science, Population Health Sciences, Food Science & Technology) whose expertise will allow SWIMM to identify needs and link developments in membrane materials and technology to specific social and environmental impacts.

New resources needed: Two primary interrelated gaps have been identified that must be filled in order to position SWIMM for national prominence. These gaps relate to the ability to transition materials and technologies from the lab scale to the pilot scale. First, only limited expertise is currently available in the area of large-scale membrane processing and manufacturing. *A targeted faculty hire, preferably at the Associate or Full Professor rank, in the area of advanced manufacturing of membranes would fill this knowledge gap*. Second, while lab scale membrane fabrication and testing facilities are available in several laboratories on campus, there are currently no larger pilot-scale facilities available. These facilities would allow the scale-up of new technologies from the lab scale (i.e., new membrane discovery) to the industrial scale, and would significantly increase VT's visibility in the area. In addition, these facilities would increase the potential for collaboration with and funding from industrial partners. It is hoped that these facilities could be developed in collaboration with the Materials SGA and IIHCC destination area.

5. Expected Outcomes

Milestones and deliverables: A significant goal of SWIMM is to foster increased interactions aimed at expanding current efforts in water purification, water quality, and membrane separations. As such, SWIMM will aim to hold quarterly meetings to generate dialog between interested faculty, as well as to identify specific opportunities for funding and outreach. These efforts will begin with a workshop this summer. We also anticipate the submission of a number of small (2-5 faculty) proposals starting in the first year of the program (e.g. NSF INFEWS, USDA-AFRI). These will be aimed at increasing collaborative research interactions between faculty across department and college boundaries.

Impact: SWIMM will impact the VT Materials community by fostering interdisciplinary collaboration and funding in the area of materials for water purification, in the hiring of a new faculty member focused on advanced manufacturing of membranes, through the development of a pilot-scale membrane fabrication and testing facility, and through the submission of numerous funding proposals culminating in Center-level proposals. These efforts will also serve to raise the national profile of VT's research efforts in sustainable water and in materials development more generally.

Appendix II: Tables and Figures

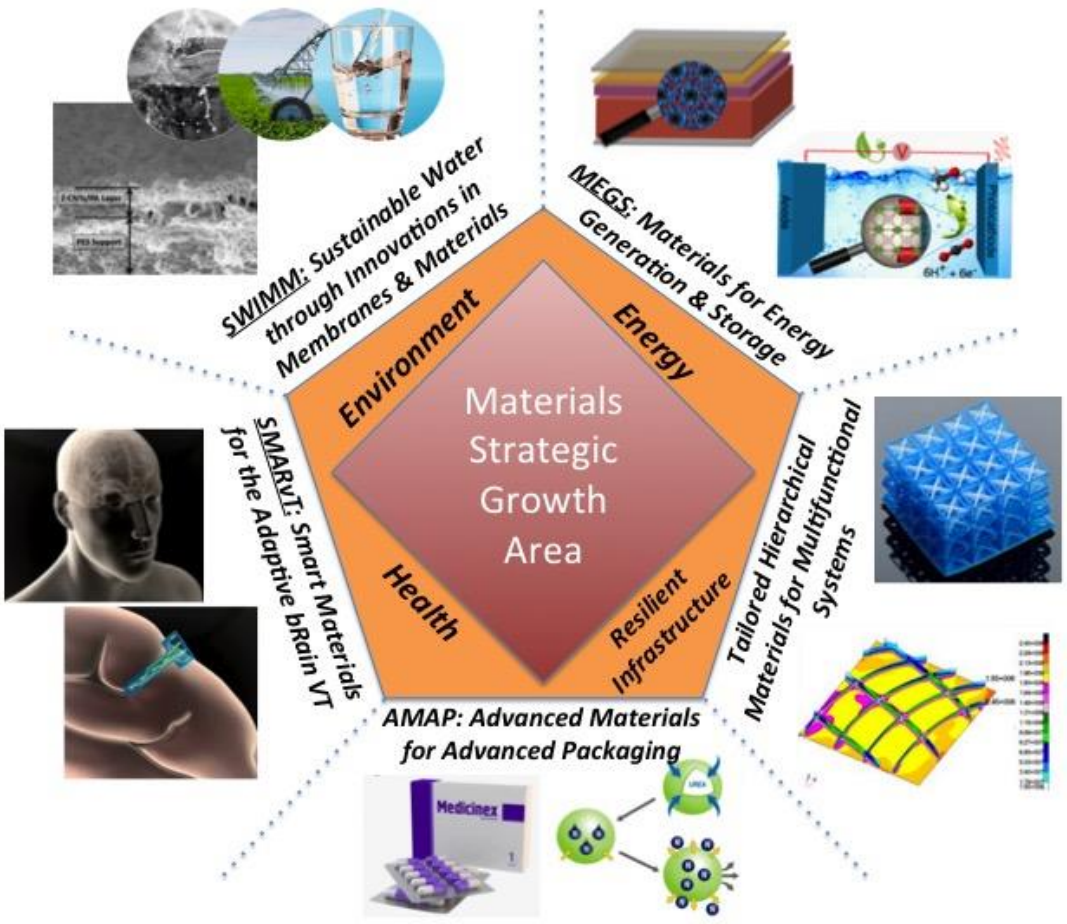

Figure 1: Materials SGA Overview

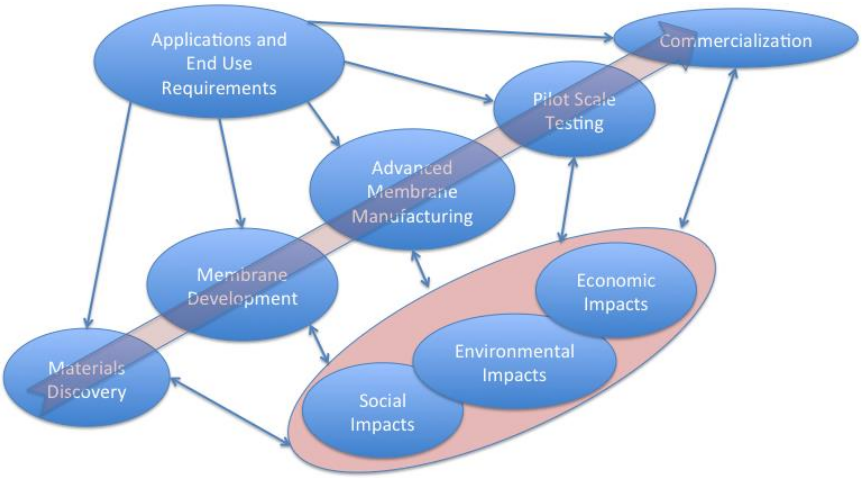

Figure 2: Sustainable Water through Innovations in Membranes & Materials - SWIMM

Figure 3: Research Team Contributions

Table 1: Milestones and Deliverables

Milestone	Deliverable	Timeline
SWIMM Workshop	Detailed report on current VT efforts and plans to interact with destination areas and other Materials SGA research pillars.	Summer 2017
New Faculty Hire	Faculty Search in the area of Advanced Manufacturing of Membranes resulting in a new faculty hire	Spring 2018
Pilot-Scale Facility	Planning and design for a combined membrane manufacturing and pilot-scale testing facility in collaboration with the new faculty hire.	Spring 2019
Center Proposal	Preparation and submission of a Center-level interdisciplinary proposal in Water Purification Membrane Materials	Fall 2020

Table 2: Team and Current Collaborations

Faculty	Department	College	Collaborations
Klaus Moeltner	Agricultural & Applied Economics	CALS	He
Brian Badgley	Crop & Soil Environmental Sciences	CALS	Dietrich, He, Stewart, Xia
Kang Xia	Crop & Soil Environmental Sciences	CALS	Steward, Badgley, Vikesland
Ryan Stewart	Crop & Soil Environmental Sciences	CALS	Long, Morris, Dietrich, Badgley, Xia
Susan Duncan	Food Science and Technology	CALS	Dietrich, Long, Hedrick, He, Edwards, Riffle
Valisa Hedrick	Human Nutrition, Foods, and Exercise	CALS	Dietrich, He
Kevin Edgar	Sustainable Biomaterials	CNRE	Martin, Moore, Long, Riffle, Baird, Foster, Cheng
David Dillard	Biomedical Engineering & Mechanics	COE	Baird, Long
Jack Lesko	Biomedical Engineering & Mechanics	COE	Riffle, Long
Donald Baird	Chemical Engineering	COE	Long, Moore, Riffle (Chemistry); Foster (MSE); Edgar (SusBio); Dillard (BEAM); Martin (CHE) - MII
Luke Achenie	Chemical Engineering	COE	Deshmukh
Sanket Deshmukh	Chemical Engineering	COE	Martin, Morris
Stephen Martin	Chemical Engineering	COE	Baird, Deshmukh, (CHE); Moore (Chemistry); Foster (MSE); Edgar (SusBio) - MII
Andrea Dietrich	Civil & Environmental Engineering	COE	Badgley, Duncan, Gohlke, He, Hedrick, Lesko, Martin, Morris, Stewart
Jason He	Civil & Environmental Engineering	COE	Morris, Badgley, Long, Dietrich, Moeltner
Marc Edwards	Civil & Environmental Engineering	COE	Vikesland, Duncan
Peter Vikesland	Civil & Environmental Engineering	COE	Edwards, Xia, He
Johan Foster	Materials Science & Engineering	COE	Martin, Baird - MII
Amanda Morris	Chemistry	COS	He, Martin
Judy Riffle	Chemistry	COS	Baird, Long, Moore, Lesko
Robert Moore	Chemistry	COS	Martin, Long, Baird, Riffle
Tim Long	Chemistry	COS	Moore (Chemistry)- MII
Shengfeng Cheng	Physics	COS	MII
Julia M. Gohlke	Population Health Sciences	Vet Med	Dietrich

Appendix III: Provisional Job Ad

Tenure Track Faculty Position
Global Systems Science Destination Area
Virginia Tech

The Global Systems Science (GSS) Destination Area at Virginia Tech seeks outstanding candidates for a tenure-track faculty opening at the rank of Associate or Full Professor. The Sustainable Water through Innovation in Membranes & Materials program (SWIMM) is an interdisciplinary research effort aimed at improving access to clean water through the development of novel materials and devices for water treatment and purification. The successful candidate should have significant experience and national recognition in the areas of advanced manufacturing and fabrication of membranes, as well as the scale-up of membrane devices and systems. The candidate is expected to take a lead role in the creation of a new membrane processing and scale-up facility on campus, and will serve as a key point of contact between other SWIMM and GSS faculty, industrial partners, and government sponsors. Applicants should have a Ph.D. in Chemical Engineering, Materials Science, or a related field, a record of excellence in research, and a commitment to teaching and working with a diverse population of undergraduate and graduate students.