Title of the area:

Non-conventional Hetero-integrated Materials for Electronics, Optoelectronics and Energy Applications

Participating disciplines/academic units/departments:

Electrical Engineering/Electrical and Computer Engineering Department

Mechanical Engineering/Mechanical Engineering and Engineering Science Department

Chemistry/Department of Chemistry

Physics/Department of Physics and Optical Science

Leads: Yong Zhang (ECE), Thomas A. Schmedake (Chem), and Terry T. Xu (MEES)

Target category:

Existing and Emerging Excellence

Key-words:

Hetero-integrated materials, Electronics, Optoelectronics, Energy, Advanced characterization

1. Executive Summary

This team has built upon one of the few historic areas of strength, microelectronics, at UNCC, and expanded into a few newer and potentially revolutionary topics, which were pioneered by some of the team members as demonstrated by the research products (journal publications and patents) of the team. These topics focus on development, basic research, and applications of smartly integrated heterogeneous materials in nanoscopic scales. They are or expected to be evolving into new research directions that will be followed by the broader material sciences and engineering community with major implications in fundamental sciences and real-world applications in electronics, optoelectronics, quantum informatics, and energy related applications.

Well-established universities have engaged in more mature material systems since the time the materials were developed decades ago. As a relatively newly established research institute, our efforts on the well-known material systems, while still necessary and meaningful, tend to yield only incremental improvement and understanding, which will not make us distinct from others. Instead, we should devote our limited resources to emerging or new material systems that can offer unique material properties, with greater tunability, and the ability to fill the critical gaps in the properties of existing materials. Our team has a well-documented record in the research related to a wide range of conventional material systems, thus we are well prepared in our efforts to explore the newly identified materials and discover additional completely new materials.

This moderate size team consists of 12 experts of diverse backgrounds in physical science and closely related areas, including physics, chemistry, electrical and mechanical engineering, who have worked together in many research projects with demonstrated close, efficient, and cohesive collaboration. These efforts have manifested as many funded/submitted/published/on-going joint proposals, journal publications, and patents. Our team also contributes greatly to the overall research reputation of our university with ongoing collaborations throughout engineering and the sciences. We contribute to the development of many other emerging areas of research excellence on campus (e.g. nanoscience, optics, bio-engineering) by providing researchers with novel materials to use, a portfolio of world-class analytical methods, device fabrication and testing capabilities, and theoretical modeling.

Relatively speaking, our university's research facility is less established compared to most R1 institutes. However, in recent years, this group of researchers have put in major effort, with great success, in improving our readiness in engaging major research projects through getting major research equipment grants and upgrading the existing instruments. We have established a number of unique material and device characterization capabilities and methodologies in individual team member's labs, in conjunction with the university wide user facility (e.g., Optics Center) and ECE cleanroom, which have positioned us as good if not better than many R1 institutes in a few key areas. The team also has the capability of performing large-scale material design and simulation using state-of-the-art software. Furthermore, we have established an international/national collaboration network to complement our capabilities.

2. Evidence of Strength and Excellence

Historically, electronic materials and devices was one of the key areas of strength at UNCC, as ECE department established one of the first three UNCC Ph.D. programs in 1993 with a research focus areas in microelectronics and optoelectronics. Semiconductor materials were the foundation and remain so for these research areas, but the scope of semiconductor materials has expanded greatly in the past few decades.

Traditional elementary and fixed-composition binary semiconductors such as Si, GaAs and more recently SiC and GaN still play the dominant roles in today's (opto)electronic related applications. In addition, semiconductors comprised of a variable composition of elements known as "alloys" for instance SiGe, InGaAs, InGaN, etc., have been developed. The primary advantage of these tunable materials is that they provide engineers the ability to design material properties that cannot be obtained by traditional semiconductors with fixed compositions.

A paradigm shift in optoelectronic occurred in 1970, when Dr. Raphael Tsu (former Distinguished Professor of ECE) and Prof. L. Esaki (Nobel laureate) proposed the first quantum mechanics level design of a hybrid structure of two materials (e.g., GaAs/AlGaAs) arranged in alternating layers of nanoscopic thickness and precision. The resulting hybrid material is often referred to as a semiconductor superlattice.[1] This invention has led to a large number of technological innovations and applications, including the widely used light-emitting diode (LED) lamps, surface-emitting lasers, and high-sensitivity light detectors, and it inspired many of the current day diverse nanoscale sciences and technologies.

Conventional wisdom would suggest to combine similar materials in terms of crystal structure and atomic size. However, the close similarity of the constituents often implies a relatively small tunability. To achieve broader material property tunability and even completely new functionalities, researchers have explored hybridization of highly dissimilar or non-conventional materials as the next generation semiconductor materials. Our group at UNC Charlotte have established excellence and international/national prominence in a few areas of this field. This is illustrated below by a few examples.

Lead PI **Y. Zhang** was one of the pioneers who started to explore a family of II-VI based organic-inorganic hybrid crystalline materials, which had led to a few high-impact publications in the field.[2-4] Recently, with co-PI **Schmedake**, they have received an AOR grant to study these materials for novel (opto)electronic applications and fundamental understanding of the design principles to achieve stable and perfect hybrid structures (a joint paper is under review). This effort could evolve into a new research frontier for developing highly stable organic-inorganic hybrid materials for applications in quantum informatics and electronics. In 2010, **Y. Zhang** and R. Tsu proposed the first superlattice structure of 2D materials (e.g., graphene/silicene),[5, 6] and demonstrated the MBE growth of ultra-thin Si layers on graphene.[7] His group subsequently collaborated with other groups (e.g., NCSU) in the study of other 2D heterostructures (e. g., MoS_2/WS_2), resulting in multiple highly cited publications.[8-13] Recently, **Y. Zhang**'s group and his collaborators (Sandia, NHMFL, etc.) reported the first observation of quantum oscillations and high mobility of a 2D electron gas at the interface of a unusual hetero-structure consisting of two semiconductors (PbTe/CdTe) with very different crystal structures.[14]

Schmedake, **Walter**, and **Y. Zhang** have a joint NSF project on the development of a novel group of Si-based organic molecules. They have had multiple joint publications, in collaboration with **Hofmann**.[15, 16] These materials have great potential for (opto)electronic applications (e.g., organic field-effect transistors (OFETs) and rare-earth-free phosphors for white-light LEDs). It has been patented and also led to the establishment of an academic spin-off start-up company, Light and Charge Solutions, LLC, which has received over $500k in non-dilutive funding to date. **Ebong** and **Y. Zhang** are collaborating in understanding the subtle role of Te clusters in the Ag based solar cell electrode,[17] and developing new Cu-based electrode material on a DOE funded project to **Ebong**. **H. Zhang** and **Y. Zhang** are collaborating on the research of MoO_3 and WO_3 nanowire structures for potential catalytic and photochromic applications.[18, 19] **Xu** and **Y. Zhang** are collaborating on the study of BC_4 nanowires for thermoelectric applications.[20-22] **Egusa**, **Bejger**, **Her**, and **Y. Zhang** are collaborating in the study of new phases of vanadium oxide for tunable and fast refractive index switching. **Y. Zhang** and **Wei** are collaborating on an exploratory research on new photochromic material, yttrium oxyhydride. **Her** and **Y. Zhang** are collaborating on non-linear optics and ultrafast time-resolved carrier dynamics of the organic-inorganic hybrid materials. **Bejger** and **Schmedake** are collaborating on studying crystalline polymers comprising transition metal chalcogenide molecular clusters for catalysis, energy storage, and electronic devices,[23-25] and **Bejger** recently received an NSF CAREER award.

Hofmann, **Egusa**, **Her**, and **Y. Zhang** are co-PIs on an NSF MRI grant for developing new material deposition capability that is much needed for transforming new materials into devices. Many of us were co-PIs on major equipment grants from ARO (one led by **Xu** – funded, one by **H. Zhang** – funded, one by **Y. Zhang** - pending), and on an NSF/MRI led by **Hofmann** (pending). **Y. Zhang**’s group has developed an array of unique microscopic scale device and material characterization techniques that have been shared with the members of this research cluster as well as many beyond this group.[26-31] The team also has the capability of performing large-scale material design and device simulation using state-of-the-art software.[32-37]

Members of this research cluster bring complementary and interdisciplinary expertise in the development, basic research, and applications of novel non-conventional materials, yet with strong background in a wide range of conventional materials.[38-45] Lead PI **Y. Zhang** has diverse external collaboration with scientists all over the world and many domestic collaborators in government labs (e.g., NREL, Sandia, LBNL, ANL, ARL, NRL, NIST) and universities. For instance, he was a co-PI on a 6-year ARO/MURI project with team members from UIUC, ASU, Georgia Tech, and TAMU; he was the lead PI on a follow-up project for a small set of the MURI team; and a co-PI on a 3-year UNC/ROI project with team member from UNC-CH, NCSU, and NCCU. Besides many high-impact journal publications, many projects led by **Y. Zhang** also received considerable medium attention (e.g., on LETs in MIT Technology Review, 2016).

Together this team has supervised 59 Ph. D and 44 MS. **Schmedake** has been running an NSF undergraduate summer research program for 13 years, hosting 130 students, with many of us as co-PIs. A majority of these 130 students come from places where research opportunities are limited or from demographic backgrounds that have historically faced societal and/or economic barriers to participation in science and engineering careers.

Often we develop new concepts and materials but are unable to effectively demonstrate their full potential due to limited resources (e. g., facility and critical mass). Advanced (opto)electronic device fabrication specifically is a weak area at UNCC. Targeted hiring in this area is requested. This strategic addition would leverage our breakthroughs in hybrid materials and properties, and in so doing would boost the overall impacts of the hybrid materials research team.

3. Alignment with Regional and National Priorities

Materials are the foundation for practically all modern technologies. We are targeting new non-conventional materials with one of these attributes: drastically improvement on key functionalities, providing currently not readily achievable properties, and low cost and environmentally friendly. For examples, our current project funded by ARO on II-VI hybrid materials are intended to achieve room-temperature exciton-polariton condensation for quantum computing, and p-type transparent conductive materials that are currently lacking for a wide range of technologies, such as PV, LED, electrochromic window; another project funded by NSF on the development of novel Si based organic molecules is seeking applications in low-cost, printable organic LEDs (OLEDs) and field-effect transistors (OFETs), phosphors in solid-state lighting to replace the commonly used phosphors based on rare-earth elements that are costly and environmentally unfriendly in production. Participation of a recently finished (2017-2020) large ROI project funded by UNC System on the development of hybrid perovskites for PV applications.

Our efforts are generally in alignment with multiple national or general science priorities, such as Growing Convergence Research and Quantum Leap among the 10 big ideas identified by NSF, Targeting Materials Science for Quantum Technologies in Quantum Frontiers: Report on Community Input to The Nation's Strategy for Quantum Information Science, multiple areas of Physical Sciences and Engineering Sciences in Army Research Office Broad Agency Announcement for Basic and Applied Scientific Research, Buildings Energy Efficiency Frontiers & Innovation Technologies in DOE Office of Energy Efficiency & Renewable Energy.

4. Supporting Documents

Table 1. Brief summary of team member information

Name	Title	Expertise
(Lead) Yong Zhang (ECE)	Bissell Distinguished Professor	Material and devices characterization; Optical spectroscopy; Electronic structure and device modeling
(Co-Lead) Thomas A. Schmedake (Chem)	Professor	Synthesis and characterization of organic-inorganic hybrid materials
(Co-Lead) Terry Xu (MEES)	Professor	Synthesis and characterization of boron-based 1D nanostructures, measurement of mechanical properties of individual nanostructures and exploration of their applications in thermoelectric energy conversion.
Christopher Bejger (Chem)	Assistant Professor	Design and synthesis of nanoclusters and redox active metal-organic frameworks.
Abasifreke Ebong (ECE)	Professor	Metal/semiconductor interface characterization for carrier transports in optoelectronic devices - solar cells, LED, photosensors, etc.
Shunji Egusa (Phys. & OS)	Assistant Professor	Nano-materials synthesis and characterization; Optical spectroscopy
Youxing Chen (MEES)	Research Assistant Professor	Microstructure - mechanical behavior correlation at the nanoscale; Interface structure characterization and the corresponding behavior under external mechanical or electric stimuli.
Wei Gao (ECE)	Cleanroom Manager, Lecturer	Semiconductor device fabrication and characterization; Cleanroom facility operation and management.
Tsinghua Her (Phys. & OS)	Associate Professor	Light-matter interaction, laser material synthesis and modification; Laser resonators and quantum electronics; Guided-wave physics; Optical sensing and metrology; Ultrafast and nonlinear optics; Nanomaterials and metamaterials.
Tino Hofmann (Phys. & OS)	Assistant Professor	Optical characterization; Advanced thin-film deposition techniques, and in-situ monitoring
Michael G. Walter (Chem)	Associate Professor	Molecular semiconductors for solar energy conversion, molecular electronics, and small molecule fluorescent biosensors.
Haitao Zhang (MEES)	Associate Professor	Materials synthesis and growth mechanism study; Structure characterization; Property measurement & testing for electronic and optoelectronic applications

(Two-page CVs for all team members are given after References)

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