Interdisciplinary Research Group (IRG) – 1: IRG – Materials for Energy

Project – 1: Multilayered, Transparent Electrodes UTEP Faculty: Dr. Ramana Chintalapalle, Mechanical Engineering

This project work will explore multilayer stacks (≤100 nm) of dielectric(D)/metal(M)/dielectric(D) films with controlled interfacial structure and chemistry. Specifically, efforts will be focused on utilizing WO_3, HfO_2 and MoO_3 for D-layers while M-interlayers will be either Ag or Al. TCOs transport photo-generated current from the active layer(s) of a device to an external load play a key role in optoelectronics (EO) and LEDs in addition to photovoltaics. Tin-doped indium oxide (ITO) is the current standard TCO for all practical applications in EO, PV and LED technologies. However, there has been much recent interest in finding indium-free TCOs and even better performing alternative candidates to substitute ITO. The driving factors, which are mainly associated with In metal, are: 1) scarcity, (2) rapid price increase, (3) unintended interfacial phenomena and (4) global politics. In addition, the poor mechanical flexibility and inevitable high deposition temperatures limit potential application of ITO in flexible and/or organic-based PV, EO and LED technologies. A large number of materials, such as metal nanowires, doped oxides, and graphene, have been extensively studied in recent years. However, none of them were found to adequately replace ITO. Recently, the concept of D/M/D multilayers has emerged as a highly promising strategy for efficient TCO design that overcomes many of the problems associated with ITO. However, the fundamental science, especially the underlying mechanism of component layers' interfacial microstructure and charge injection mechanisms are not well understood at this time. In this context, **the project will** investigate the fundamental science and engineering aspects of TCOs based on D/M/D multilayer films. The technical merit of the project is to use an asymmetric configuration, where the top and bottom D-layers are materials with different refractive index (such as WO_3 and HfO_2), which is expected to significantly improve the electronic behavior to meet the ideal requirements of TCOs. Therefore, experiments will be performed to understand the effect of various morphologies on the DMD-TCOs performance. D/M/D as well as other transparent oxide materials will be deposited using standard physical vapor deposition methods, such as sputtering, electron-beam deposition, and pulsed-laser deposition, under variable conditions of temperature, oxygen reactive pressure and D/M-layer thickness. The samples will be characterized by studying their crystal structure, surface/interface structure and morphology, chemical composition, and optical and electrical measurements. The structural and chemical characterization of the samples will be performed employing X-ray diffraction (XRD), Xray reflectivity, scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS) measurements. The electrical properties of D/M/D samples will be measured employing the van der Pauw method while the optical properties will be probed employing spectrophotometry and spectroscopic ellipsometry (SE).

Project – 2: Uranium-Based Compounds for Energy Applications UTEP Faculty: Dr. Skye Fortier, Chemistry

The use of unconventional uranium ceramics may give access to new photovoltaic materials or devices. Indeed, uranium oxide based, thin-film solar cells have been patented, demonstrating proof of concept. The problem with these materials is that they are difficult to make owing to their high melting point (e.g. UO_2, m.p. 3,138 K) which complicates growing well-defined films or crystalline solids. Moreover, computational modeling of the local bonding interactions in the ceramics between uranium and the interstitial atom can be complicated due to 5*f*-electron relativistic effects, hindering critical understanding of the underlying chemistry.

In an effort to advance the use of uranium materials in energy applications, particularly in light harvesting devices, we propose to take a multi-prong approach. Specifically: a) new methods

for the deposition of UO_2 ceramic films and single crystals will be explored; b) the physical properties of these materials in devices will be investigated.

While the role of uranium ceramics has been the focus of study for several decades, owing to their importance in the nuclear fuel cycle, very little work has been performed in applying their unique properties to conducting materials. UO_2 is a semiconducting ceramic with an electronic bandgap of 1.3 eV, lying in-between Si (1.14 eV) and GaAs (1.39 eV), with a high dielectric constant of 22 at 300 K. Moreover, at room temperature, the intrinsic electrical conductivity of UO_2 is comparable to that of crystalline Si. The semiconducting behavior can be explained by unique 5*f*-electron-hopping using a Hubbard exciton model. UO_2 also has potential utility as a thermoelectric material as it exhibits a high Seebeck coefficient of 750 μV/K (320 K, 0.01 W/cm□K). The lack of study in this area is less likely a result of radioactivity (U is a weak α-emitter) and more a consequence of high-temperature synthesis of the refractory uranium ceramics.

The deposition of metal oxides via sol-gel methods is a well-established technique. The **Fortier** laboratory is working to extend this method to uranium as a low-temperature route to UO_2 thin film formation. To achieve this, the ditox ligand (ditox = $^{-}OCH^{t}Bu_2$) was chosen as it is both bulky and anticipated to provide high solubility in a wide range of solvents, thus conferring kinetic stability to the complex and ease of handling and processing.

Project – 3: Multifunctional Materials for Energy Harvesting Applications UTEP Faculty: Dr. Ramana Chintalapalle (Mechanical Engineering) and Dr. Chunquiang Li (Physics)

Multifunctional materials, which can combine multiple properties and phenomena in the solid state, find numerous technological applications. The perovskite (ABO_3) structured $BaTiO_3$, which is a classical ferroelectric (FE), and BTO-based solid solutions are an important class of materials that are useful for many of the current and emerging technological applications. $BaTiO_3$ and BTObased materials are of great practical interest due to their excellent properties such as relatively high stability, high dielectric constant (ε' ~1700), low dielectric loss (tan δ~0.01), and moderately high piezoelectric coefficient (d_{33}~150 pC/N). We propose to use non-magnetic (NM) Ce and Sn ions for incorporation into Ca-doped BTO to tune the structure, chemistry and physical properties. To produce the electronic structure changes, suitable ions must be doped at the Ti(B)-site that induce significant changes in the electronic structure (to facilitate charge carrier generation) while still maintaining the ferroelectric signature (to facilitate the charge transport) of BTO. From fundamental scientific perspective, doping at B-site by suitable metal ion(s) can induce changes in the octahedral ordering and local bonding, and thus facilitates the E_g-reduction. The substitution of Ti^{4+} by slightly larger Sn^{4+} and/or Ce is expected to induce such changes leading to unit cell expansion and property modification. The central theme and fundamental scientific aspects of the proposed research are to gain an insightful understanding of the structure-property-processing relationship, which can help in substantially advancing our fundamental understanding while elucidating the role of dopants on the properties.

Interdisciplinary Research Group (IRG) – 2: IRG – Bio-Materials

Interdisciplinary Research Group (IRG) – 2: IRG - Biomaterials

Project – 4: Development of An Extrusion-Based 3D-Printing Strategy for Culture of Human Neural Progenitor Cells

UTEP Faculty: 1. Dr. Binata Joddar (Metallurgical, Materials and Biomedical Engineering)

Cells have traditionally been studied under 2D culture conditions, by growing cells directly on the surface of cultureware. However, a 3D environment can more closely mimic conditions in the body, providing greater structural complexity and facilitating cell-cell interactions observed in human tissue1 . One method of growing cells in a 3D environment is to encapsulate the cells in a biocompatible gel-like material called a “bioink,” and then use a 3D bio-printer to print the cell and bioink mixture into the desired structure. Hydrogels, made of crosslinked hydrophilic polymer chains, are often used as a “bioink” in 3D bioprinting. Their physical properties can be tuned to emulate specific types of tissue, but formulating hydrogels for cell survival while retaining printability is a major challenge. In this study, a highly viscous hydrogel was needed for compatibility with the extrusion-based 3D bioprinting system used. In extrusion bioprinting, the printer applies pressure to extrude bioink through a small nozzle. In our experiment, we assessed the viability of human neural progenitor cells (NPCs) in 3D structures printed with a hydrogel bioink formulation, previously optimized by University of Victoria (UVIC) collaborators for neural cell growth2, and subsequently modified for structural support during extrusion bioprinting. Previous studies3 have shown that growth of cardiomyocytes can be supported in a 3D bioink. We have chosen to work with NPCs to begin developing a platform that is compatible with both cardiomyocytes and NPCs, and could be used to study interactions between the cells of the human brain and heart. Our objective of the research is to determine whether human neural progenitor cells (NPCs) could be successfully cultured in 3D structures made of a hydrogel mixture optimized for both cell proliferation and extrusion bioprinting.

Project – 5: Photothermal Nanomaterials for High-Efficiency Biomass Conversion

UTEP Faculty: Dr. Xiujun (James) Li, Chemistry

To address the low-efficiency problem of biomass conversion, this team will systematically study fundamentals of the localized heat of photothermal effects of a variety of nanomaterials for efficient biomass conversion. The central hypothesis is that localized heat generated from the nanomaterial-medicated photothermal effect on the catalyst surface can significantly increase the catalytic efficiency. The team members will work synergistically on various aspects, which include nanomaterial and nanocomposite synthesis, characterization, photothermal effects, biomass conversion efficiency and catalytic synthesis, *modeling,* kinetics and mechanisms.

Conversion of plant-based biomass into valuable biofuels and fine chemicals has gained increasing significance due to the growing demand for renewable energy and materials. Through the biomass conversion of cellulose and related carbohydrates, many value-added chemicals can be produced. 5-(Hydroxymethyl)furfural (**HMF**) is one of such examples. HMF upon oxidation yields 2, 5-furandicarboxylic acid (**FDCA**), which is one of the most important bio-renewable alternatives to terephthalic acid and starting chemicals for the manufacturing of petroleum-based polymers such as polyethylene terephthalate (PET) and polybutyleneterephthalate (PBT) plastics. However, current methods for the oxidation of HMF into FDCA are of low efficiency and dependent on lengthy reaction time, high pressures, and toxic catalysts.[63,64-65] Exploration of new methods for efficient biomass conversion becomes vital to the production of valuable materials from biomass resources.

Although photothermal effect is extensively studied for cancer photothermal therapy due to its unique noninvasive characteristics, it is rarely studied for biomass conversion. One of the key attributes of photothermal effect is its ability to cleave strong chemical bonds rapidly from **localized heat** generated from the surface plasmon resonance of nanoparticles. Further, when utilized in catalysis, this localized heat can aid in more rapid conversion of reactants than the heat supplied externally to the reaction medium, thus dramatically improving the catalytic efficiency of biomass conversion. Our preliminary studies show a photothermal method (at 60 ºC, in a bulk solution) can lead to 400% enhancement in the time required for >99% conversion of HMF, compared with the same HMF oxidation process at 60 ºC by conventional heating of bulk solutions, while more than **70-fold enhancement** was observed when compared with the room

temperature method. Different gold nanoparticles, nanorods and nanoshells were observed to have catalytic effects in biomass conversion. Because those nanomaterials also have good photothermal effects, this **dual effect (localized heat** and their **catalytic effect)** can significantly increase the biomass conversion efficiency. The majority of the existing reports on photothermal effects focus on gold nanoparticles. Some the photothermal effects of other nanomaterials such as the porous gold nanosponge (**PGN**) and nanocomposites were never reported. Systematic studies of photothermal effects of different nanomaterials are expected to provide fundamental scientific clues to dramatically improve the biomass conversion.

Project 6: AI/ML for Molecular Discovery and Property Prediction
UTEP Faculty: Dr. Suman Sirimulla (School of Pharmaceutical Sciences)

The proposed project is intended to design, conceptualize, characterize, and demonstrate the novel chemical molecules, which can ultimately serve in fthe treatment of dangerous infectious diseases. For instance, currently, novel coronavirus (SARS-CoV2) infections have been spread all over the world and causing devastating effects. Previously other viruses such as MARS, SARS, and Ebola also had a severe impact on public health. Currently, there are no approved therapies for the treatment of novel coronavirus disease (COVID19). Currently, the chemical space for drug discovery (potential drug-like compounds) is estimated to be around 10^{30} to 10^{60} compounds. We hypothesize that searching vast chemical space would help find potent and chemically diverse inhibitors. Therefore, the overarching goal of this proposed work is to explore the vast chemical space to find potent inhibitors of viral proteins that are involved in SARS-CoV2 replication. We will rely on two strategies to implement our approach and achieve success. The two strategies are: 1) use an inverse molecular design approach that can produce molecules with optimized desired properties, 2) virtually screening the vast chemical space of 1.4 Billion compound make on demand library against multiple viral proteins. The specific objectives of the proposed project are as follows.

The goal objective is to design set of potential antiviral molecules, which would be synthetically accessible, have a drug-like properties, and possess chemical diversity. Screening several billions of molecules using a virtual screening is computationally very expensive. Thus, we hypothesize that an inverse molecular design approach that can produce molecules with desirable properties can be better. Towards this end, first, we will design an AI engine that will create molecules of interest. We will employ the cutting-edge artificial intelligence (AI) algorithms combined with knowledge of existing chemical molecules and synthetic strategies to design the software. In particular, we will utilize Transformer neural network architecture, which has proven results in the neural machine translation and image captioning, to generate novel chemical matter that is likely to act against viral proteins. Transformer models use the self-attention mechanism that yields a probability distribution over each element in the vocabulary for each position in the output sequence. The mechanism refers to different components of a single sequence in relation to other components to compute sequence representation. Therefore, it allows capturing long-range dependencies between items in sequence and enables the networks to learn semantic and synthetic properties of drug compounds from a fundamental chemistry perspective. As a result, these models generate realistic diverse chemical compounds with diverse structural novelty. We will also systematically evaluate the performance of transformer-based neural networks with other state-of-art generative models in developing new chemical molecules/matter. By using this novel approach, we will create a small set of molecules that will likely inhibit non-structural viral proteins that are involved in the viral replication process of COVID-19.

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