Taiwan lacks natural resources and thus sustainability becomes extremely crucial. In order to comply with Taiwan's New Energy Policy, which is to reduce CO₂ emissions (regarded as the main cause of global warming and environmental pollution resulting from burning fossil fuel), green alternative renewable energy must be a top priority. In order to harness the full capacities of renewable energy sources, e.g., solar and wind power which are inherently intermittent, clean and sustainable energy storage is undoubtedly needed. Grid-scale energy storage is emerging as one of the largest potential applications for electrochemical devices and will require abundant, low-cost, ultra-stable electrodes. Increasing needs in high energy density and limited excess to lithium resources will require the discovery of new electrochemistry beyond lithium technology. New rechargeable battery systems based on multivalent cation charge carriers, such as Mg²⁺, Zn²⁺, Ca²⁺, and Al³⁺ ions, which involve more than one electron transfer, have the promise to deliver higher specific capacity and energy density. However, in order to materialize these new energy storage technologies, several challenges must be overcome. The objective of my project is to design and develop advanced functional materials with complex nanostructures as electrode materials and solid-state electrolytes, which are the two most important components affecting the properties and electrochemical performance of high energy-density multivalent-ion batteries. My interests concern three distinct yet related areas: (1) conductive porous metal-organic frameworks for electrochemical energy storage, (2) conductive polymeric porous materials as battery electrodes, and (3) surface engineered materials for better electrochemical performance. The findings from this project will address a broad range of research challenges, from new materials discovery to energy storage. My research will uncover the relationships between materials properties, electrode architectures, and electrochemical mechanisms. I feel tremendously honored to be a MOST grant recipient for the Einstein Program to pursue this project. None of this would be possible without the support from Taiwan Ministry of Science and Technology (MOST). I have been fortunate to have great support from National Cheng Kung University. I sincerely thank all my wonderful colleagues at the Department of Chemical Engineering for their generous guidance.
Most Young Scholars Grant (Einstein Program): Exploring New Possibilities – Role of Complex Oxides

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Oxide materials are gifted systems which have attracted lots of attention over past decades. These materials provide a variety of intriguing functional properties, including superconducting, piezo/ferroelectric, magnetic, high-dielectricity, ferromagnetism, colossal magnetoresistance, transparent-conducting and etc., where typical examples and configurations are listed in Fig. 1. With proper control, the interplays between charge, lattice, orbital and spin degrees of freedom in complex oxides enable us to design materials with new functionalities. The fundamental understanding of the physical origin of these phenomena is crucial in order to develop the principles for materials design and to exploit the remarkable properties of these materials for new practical devices.

Prof. Jan-Chi Yang established the laser molecular beam epitaxy (Laser-MBE) lab at Department of Physics since August 2017. He is an experimental researcher who is highly interested in understanding complex phenomena in novel materials of fundamental and/or technological importance with the aid of multiple complementary experimental techniques. He believes that the scientists have great potentials to fundamentally change our view of the modern world, to significantly impact the technology, and to provide new solutions to our energy issues. In the past years, he mainly focuses on the growth and creation of functional materials, interfaces, heterostructures, nanostructures and free-standing matters via laser-MBE techniques, and recently he’s trying to use the synchrotron-based techniques and transport measurements to reveal the answers to the charming and fascinating physics in quantum materials. His main goal is to strike an elegant balance between physics and materials science for creating new quantum materials with new functionalities and for unveiling the intriguing interplays more comprehended. His papers have been published in Nature Commun., Phys. Rev. Lett., Advanced Mater., ACS Nano, Nano Letters, PRB, and so on. In 2018, he was awarded the Einstein program, founded by Ministry of Science and Technology (MOST).
Laser-MBE lab was found to tackle various problems arising under the above research themes using the various techniques. The advanced growth of functional materials has played an important role to initiate the bloom of green electronics and novel applications. Fig. 2 shows the initial setup of Prof. Jan-Chi Yang’s group. In the foreseeable future, he plans to combine his expertise in advanced growth, synchrotron-based techniques as well as transport measurements to study and to develop new complex oxides, especially fascinating oxide homo-, hetero- and nano-structures. Laser-MBE lab is also open for collaboration in developing intriguing physics and functionalities in new materials.

Fig. 2 Lab setup of Laser-MBE lab at Department of Physics, NCKU.
Most Young Scholars Grant (Columbus Program) -- Privacy-preserving Social Data Mining with Its Applications

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Online social platforms such as Facebook and Twitter allow users to interact with not only each other, but also a variety of entities via a rich set of social functions. Users can rate items, follow one another, check-in at places, and generate posts with hashtags. Although such heterogeneous social interaction data enrich user experiences and boost the profits of service providers and advertisers, they also bring privacy risk of users. The adversary can leverage artificial intelligence techniques to predict users’ visited locations based on hashtags, infer users’ rating preferences and purchasing habits, and identify the personal attributes and friends of users using the shared posts with check-in records. In this MOST Columbus Project, we aim at developing a general-purpose privacy-preserving framework based on online massive social datasets by exploiting and developing the techniques of machine learning, social network analysis, information security, and text mining. The ultimate goal is to simultaneously protect user privacy of sensitive data, and ensure data usability in various applications of data science.

The potential technique contribution of this project is three-fold, privacy-preserving machine learning algorithms, secure distributed social recommender systems, and information diffusion-based privacy prediction shielding methods. This project will also generate multifaceted profits. Users are allowed to experience secure online social services. Service providers with accurate and privacy-protected recommendation can boost traffic flow while lowering down the cost. And advertisers will raise the monetary income without leaking personal data.

The research interests of Prof. Li include data mining, machine learning, social network analysis, and recommender systems. Prof. Li would like to express his deep appreciation to the help from different units of NCKU. He sincerely thank for the support and encouragement of Departments of Statistics, Department of CSIE, and Institute of Data Science. Prof. Li expected to contribute himself for promoting NCKU’s data science in relevant international research communities, and to cultivate talents of data science and artificial intelligence to serve the society.
Most Young Scholars Grant (Columbus Program): A Systematic Investigation of the Structure, Function, and Regulation of Phytohormone ABC Transporters

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Plant hormones are similar to hormones in animals. They have to be delivered to the proper tissue site through a series of sophisticated transport mechanisms after being synthesized at another tissue site. Then, these plant hormones can function as the signaling molecules to induce the proper physiological response. Therefore, there are a series of active transport proteins that can regulate the distribution of phytohormone in plants. These proteins belong to ATP-binding cassette transporter (ABC transporter) family which could hydrolyze ATP as the energy source to accelerate the translocation of substrates across cell membranes. Several ABC transporters have been found to deliver the corresponding phytohormones, including auxins, abscisic acids, cytokinins, strigolactones and jasmonic acids. However, there is still a lack of biochemical studies on these phytohormone transporters. Especially in the protein structural studies, no related structure has been published so far. Exploring the biochemical properties, the functional structure and the regulatory mechanisms of these transporters, would be very helpful to clarify their role in plant physiology, as well as to elucidate their working mechanism. Therefore, we have proposed a five-year research project to conduct a comprehensive investigation on the biochemical functions, molecular structures and regulatory mechanisms of these phytohormone transport proteins. Based on our past experience in X-ray crystallography and the expertise of our international partner, Dr. Kuang-Lei Tsai, in cryogenic electron microscopy, we will utilize multiple cutting-edge biophysical approaches to study these important topics in plant physiology.

I am very thankful to have received the MOST Grant for my research project. First of all, I would like to thank the Ministry of Science and Technology for their trust and support for young scholars as well as the hard work of all the review panel members. I’m also very grateful to have many suggestions from senior professors during writing this proposal. More importantly, I want to thank National Cheng Kung University to provide the excellent research environment and all aspects of administrative support. It is my pleasure to have the opportunity doing some challenging works for NCKU and Taiwan. However, I also feel a deep responsibility for making this project is well conducted. In the future, I will do my best to learn and work with my team for making some contribution to the scientific and technological development in Taiwan.
Most Young Scholars Grant (Columbus Program) : Innovative technology research: mitigating landslide damage under extreme conditions

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Continuous global environmental change, leading to extreme rainfall and frequent earthquakes, has played a pivotal role in recent geohazard activities, and the associated landslides and disasters would cause damages directly/indirectly. Notice that extreme events are becoming the new normal, geohazard activities will become more frequent and disruptive. Analyses of landslides under the condition of extreme events will require hybrid approaches and rely on refined information and quality data. The break points include: 1) emphasize the initiation time to landslide events and locate it precisely; 2) define Taiwan mudstone failures and promote it to be internationally recognized; 3) leverage experimental tools via innovative ideas and new applications. To expand the scope of the work, development and advancement of disaster prevention technologies will also part of the achievements. It is hoped that the work may shed new lights internationally and solve geohazard challenges faced in Taiwan.

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I thankful to the President of NCKU, mentors, and colleagues for their kind encouragements and very generous supports. It is because of their guidance and sharing I am able to see further. Teaching benefits teachers as well as students; I appreciate all kinds of involvements and interactions with students very much, which certainly enabled me to think differently. Last but not least, I am most grateful to the reviewers, MOST, and our beautiful Taiwan for cultivating me with opportunities. I dedicate all honor to the National Cheng Kung University with my sincere gratitude and respect.
Most Young Scholars Grant (Columbus Program): A Dopingless Transistor

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By adopting the charge-plasma concept, dopingless FETs with metal-semiconductor (MS) and metal-insulator-semiconductor (MIS) contacts in parallel at the source/drain (SD) have been studied in this work. It is found that currents may be mainly pathing through the MIS contacts for a given SD metal workfunction when the insulator thickness is thin enough. In order to avoid the potential penalty caused by Fermi level pinning, the dopingless FET with merely SD MIS contacts has been proposed as well. The impacts of insulator material parameters on the electrical characteristics of the dopingless FET, such as bandgap, electron affinity, dielectric constant and physical thickness, have been investigated systematically. Based on numerical simulations, this work provides a general guideline with physical insights for designing dopingless FETs with high-permittivity insulator at the SD MIS contacts.

The proposed device (Fig. 1) with an active dopingless Si surrounded entirely by thin insulators features merely MIS contacts at SD, and which can be formed precisely by the atomic layer deposition in real process. Two adjustable metal workfunction at SD ($WF_{SD}$) and gate ($WF_G$) are specified in simulations. The gate electrode is isolated from SD by a distance of 5 nm, and which can be achieved by the spacer formation in real process. Variable Si body thickness $T$ and insulator thickness $t$ are used to investigate their impacts on the electrical characteristics of the devices. To mimic the reality, the Si background doping concentration is specified at $1\times10^{15}$ cm$^{-3}$, instead of the theoretical value of $1\times10^{10}$ cm$^{-3}$ at room temperature. Note that all results show in this work would not be changed obviously by the background doping ranging from $1\times10^{10}$ to $1\times10^{17}$ cm$^{-3}$.

The electrical characteristics are computed by solving the Poisson and continuity equations self-consistently involving a quantum correction model to consider the carrier redistribution near the insulator interface. Physical models include nonlocal band-to-band tunneling and nonlocal tunneling through insulating and Schottky barriers. The tunneling probability of the nonlocal tunneling models is calculated based on the WKB (Wentzel-Kramers-Brillouin) approximation of the electron wavefunction. Note that the gate tunneling leakage current has been excluded in simulations because it can be a valid assumption when a high-k metal gate stack is employed in real process. Phonon-limited bulk carrier mobility, carrier velocity saturation and Shockley-Read-Hall generation are considered as well.

Though MIGS is not considered directly, its consequence, namely effective $WF_{SD}$ due to FLP, is a variable in simulations. With this approach, the electrical performance of the device in Fig. 1 will be enhanced when the workfunction is depinned and approaching to an ideal value, such as low $WF_{SD} \sim 4.0$ eV for n-channel. Note that Si electron affinity $\chi_e = 4.05$ eV, dielectric constant $\varepsilon = 11.9$ and $E_g = 1.12$ eV are specified in all simulations.
Impacts of the insulator material parameters, such as \( t \), \( k \) and \( E_g \) and \( \chi_e \), on the electrical characteristics of the proposed device are exhibited in Fig. 2(a-c), respectively. A thinner \( t \) promises higher \( I_{DS} \) by lowering the effective tunneling resistance at MIS contacts (Fig. 2(a)). A higher \( k \) value of the insulator at the MIS contact enhances the on-current (Fig. 2(b)), and which can be explained by the higher induced electron density in a wider area benefiting the carrier conduction. For a given \( WF_{SD} \), on the other hand, if insulator \( E_g \) is decreased by rising its valence band edge, no difference on the electrical characteristics is observed (not shown). It is due to the fact that the electron tunneling probability is a function of barrier height \( \phi \) between the metal \( WF_{SD} \) and insulator \( \chi_e \) at the source MIS contact (between the semiconductor and insulator \( \chi_e \) at the drain MIS contact). Therefore, Fig. 2(c) shows the transfer characteristics for different \( \phi \) and \( t \) with a given \( WF_{SD} \). The on-current increases with decreasing \( \phi \) due to higher tunneling probability, and the enhancement is less obvious for a thinner \( t \). In addition, the on-currents also exhibit strong dependence on \( \phi \) by changing \( WF_{SD} \) (Fig. 2(d)) for the same reason.

Fig. 2. Transfer characteristics of dopingless Si FETs (Fig. 1) with different (a) \( t \), (b) \( k \), (c) \( \phi \) and (d) \( WF_{SD} \) at the MIS contacts. Besides those specified in the legends, the material parameters of the insulator (SiO\(_2\)) are specified by: \( \varepsilon = 3.9 \), \( E_g = 9 \) eV and \( \chi_e = 0.9 \) eV. The curve with \( k = 17 \) in (b) has been shifted by +50 mV for a clear comparison.
Dopingless Si FETs with MS and MIS in parallel and with MIS only at SD contacts have been studied. It is found that if MS and MIS contacts are in parallel, currents may be mainly pathing through the MIS contacts for a given SD metal workfunction when the insulator thickness is thin enough. For the proposed device with MIS SD contacts only, the on-current can be improved by reducing the physical thickness, lowering the potential barrier height and increasing the dielectric constant of the insulator at the MIS contact. A lower effective $WF_{SD}$ would boost the on-current by increasing electron tunneling probability at MIS contact as well, and which is achievable in reality by an insulator depinning the metal Fermi level for dopingless Si. In addition, it is also found that a thicker dopingless Si body increases the off-current owing to the loss of gate controllability in depth. This work combines the charge plasma concept in dopingless semiconductor and MIS ohmic contact, and predicts the electrical characteristics of the proposed device. It provides a general guideline with physical insights for designing dopingless FETs with high-k insulator at the SD MIS contacts.

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Most Young Scholars Grant (Columbus Program) : Investigating the novel topological electronic structures and spectroscopy simulation

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In traditional materials, insulators and metals are two entirely different material phases, but the bulk insulating and surface metallic properties are coexistence in topological material (Figure 1). This exotic electronic structure not only display rich fundamental physics but also provide possible applications in next generation electric devices, such as dissipationless spin current and quantum computations. Recently, our research group successfully predicted the novel topological phases in much different kind of materials of various dimension, relying on the combined methods of first-principles calculations and theoretical modeling. In the next step, we are going to simulate spectroscopy experiment, directly to provide the required experimental parameters and the results of the signal. This research is expected to greatly reduce the experimental cost of synchrotron radiation source and related experimental equipment. Besides, we will construct material database and develop machine learning to search entirely new materials that never been synthetized previously. The success of this proposal will lead to the historic breakthrough not only on the understanding of fundamental physics but also on developing and designing future device applications.

Figure 1: The schematic band structure of topological material.