<u>Workshop on advanced energy materials and x-ray spectroscopy</u>

<u>新穎能源材料暨 X 光光譜學研討會</u>

Program

Time\Date	5/4 (三)	Chair	Time\Date	5/5 (四)	Chair
08:40-09:10	Registration		08:40-09:10	Registration	
09:10-09:20	Opening Zhong/Du		09:10-09:40	Ying-Chih Pu	***Chuang***
09:20-10:00	Liejin Guo	***Du***	09:40-10:10	Chen-Hao Wang	
10:00-10:30	Jun Zhong		**10:10-10:30**	**Coffee Break**	
10:30-10:50	**Coffee Break**		10:30-11:00	Wensheng Yan	***Hsueh***
10:50-11:30	Lionel Vayssieres	***Dong***	11:00-11:30	Hengxing Ji	
11:30-12:00	Ping-Hung Yeh		11:30-12:00	Cheng-Hao Chuang	
12:00-13:40	**Lunch**		12:00-**Lunch**		
13:40-14:20	Shaohua Shen	***Yeh***			
14:20-14:50	Chin-Jung Lin				
14:50-15:20	Te-Wei Chiu				
15:20-15:50	**Coffee Break**				
15:50-16:30	Di-Jing Huang	***Pong***			
16:30-17:00	Yu-Shan Huang				
17:00-17:30	Ching-Shun Ku				
18:30-	**Banquet**				

Solar Hydrogen: Harvesting Light and Heat from Sun

Liejin Guo

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My research group in the State Key Laboratory of Multiphase Flow in Power Engineering (SKLMF), Xi’an Jiaotong University has been focusing on renewable energy, especially solar hydrogen, for about 20 years. In this presentation, I will present the most recent progress in our group on solar hydrogen production using light and heat. Firstly, “cheap” photoelectrochemical and photocatalytic water splitting, including both nanostructured materials and pilot-scale demonstration in our group for light-driven solar hydrogen (artificial photosynthesis) will be introduced. Then I will make a deep introduction to the achievement on the thermal-driven solar hydrogen, i.e., biomass/coal gasification in supercritical water for large-scale and low-cost hydrogen production using concentrated solar light.

Hematite nanostructures for efficient solar water splitting

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Hematite has emerged as a good photocatalyst for solar water splitting but the current performance of hematite is still far away from the ideal case due to various factors. Many efforts have been taken to improve the performance of hematite and Ti-based treatments have been widely used and considered to be very effective methods. However, the mechanism of Ti-based treatments is still under debate. Here we show two facile Ti-based treatments of hematite which result in a significant enhancement in photocurrent density (2.0 mA/cm^2 at 1.23 V *vs.* RHE) compared to that of the pristine hematite. The performance of the product can be further improved by coupling with Co-Pi catalysts, achieving a high photocurrent of 2.6 mA/cm^2 at 1.23 V *vs.* RHE. Our facile Ti-treatment with high photocurrent stands for an effective method to improve the performance of hematite. Moreover, synchrotron-based soft X-ray absorption spectroscopy analyses clearly revealed the formation of Fe_2TiO_5 structure on hematite after different Ti-based treatments, which reduced the photo-generated hole accumulation and then improved the performance. The formation of the Fe_2TiO_5-hematite heterostructure can also be applied to understand the enhanced performance of other Ti-treatment processes in the literature and may provide resolution of the longstanding debate regarding the mechanism of Ti-based treatments.

Interfacial & confinement effects in oxide semiconductors

Lionel Vayssieres

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The cost-effective and efficient generation of renewable fuels such as hydrogen is crucial to ensure a sustainable future where energy production for industrial development becomes respectful of the environment, biodiversity and public health. Hydrogen generation using the two most abundant and geographically-balanced natural free resources, that is seawater and solar energy can fulfill such crucial requirements. The latest achievements in quantum confinement effects and interfacial electronic structure engineering of metal oxide heteronanostructures will be revealed. Quantum dot-sensitized hematite quantum rod-arrays with full visible-light absorption profile due to intermediate band and stable against photo-corrosion for low cost solar hydrogen generation by direct water splitting at neutral pH will be demonstrated. Moreover, controlled size effects on the surface chemistry, bandgap, band edges, orbital character, and electrical conductivity as well as the experimental observation of spontaneous electron enrichment of metal *d* orbitals in oxide heteronanostructures will be presented along with a novel approach based on spontaneous photoelectric-field enhancement to fabricate highly ordered hybrid molecular-inorganic semiconductor materials and latest materials discovery for highly efficient solar energy conversion and water oxidation will be demonstrated.

Metal oxide nanostructures applications

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The UV detection ability of metal oxide nanosensors will be affected by the surrounding gas condition, charged gas/bio-molecules induced surface/interface band bending of the metal oxide nanostructures. Integrating the optical analysis into electrical measurement system for nanodevices detection analysis, the sensing mechanism of photodetector and gas/bio-detectors can be studied and clarified from the PL and Raman spectrum analysis.

1D Metal Oxides for Solar Water Splitting

Shaohua Shen

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In the past decades, numerous semiconducting materials, especially oxide semiconductors, have been investigated as potential photoelectrodes in photoelectrochemical (PEC) system with a view to efficient light-induced water splitting for solar-hydrogen conversion. Compared to other metal oxide semiconductors, α-Fe_2O_3 (hematite) has the advantage such as the small band gap energy of ~2.0 eV, which enables it to absorb most of the photons of solar spectrum. Unfortunately, the ultrafast recombination of the photogenerated carriers and the poor minority charge carrier mobility lead to a short hole diffusion length in α-Fe_2O_3, which severely limits the overall photocurrents produced by solar light. ZnO, as a wide band gap semiconductor, has many attractive material properties, including non-toxicity, low cost, large excitation binding energy, high electronic conductivity. However, either ZnO particles or nanostructured ZnO films have a wide band gap of ~3.2 eV, suggesting that only ultraviolet (UV) light could be utilized. Effective and controlled doping with metal or non-metal ions is a very common method to modify the electronic and optical properties for metal oxides semiconductors. It was demonstrated that engineered doping with metal or nonmetal ions displayed positive effects on the efficiency of α-Fe_2O_3 and ZnO nanorod photoanodes. In this presentation, some successful examples of engineered doping (Ta bulk doping, Ag surface engineering and N gradient doping) will be introduced, and related mechanisms for enhanced PEC water splitting will be discussed in detail.

CO_2 capture using chemical loop of mesoporous CaO/SiO_2 spheres obtained from agricultural wastes

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Calcium looping process (CLP) is a CO_2 capture scheme using solid CaO-based sorbents to remove CO_2 from the power generation and H_2 -production plants, producing a concentrated stream of CO_2 suitable for storage. However, the rate of carbonation of CaO makes a transition from a fast to a very slow diffusion-controlled rate. We combined the wet chemical route with an aerosol-assisted self-assembly process to prepare mesostructured CaO/SiO_2 spheres with high surface area and crystallinity for CO_2 capture through calcium looping process. The obtained adsorbents were characterized by SEM, TEM, and EDS. The CO_2 capture capacities and CLP stability were evaluated in thermogravimetric analyzer under the simulated fuel gas. In addition to advancing the support, this study provided another cost-efficient and general approach to design high performance CO_2 solid sorbents for post-combustion capture technologies.

Nobel Functions of Delafossite Materials

Te-Wei Chiu

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Cu-base Delafossite $CuMO_2$ (M = Al, Cr, Fe) has attracted much attention as a p-type transparent conductive oxide (TCO), which is of great interest for several applications such as transparent diodes and solar cells. Related studies on delafossite oxides are interested not only in examining the TCOs properties but also in exploring their applications as photo catalysts for hydrogen evolution and NO_2 removal, catalysts for steam reforming process and exhaust gas purification, room temperature ozone sensors, magnetics, and thermoelectric devices.

One way to improve the catalysis efficiency is to decrease the size of the catalyst in order to increase the surface area and adsorption ability. Synthesizing nanosized $CuCrO_2$ powder can therefore be expected to improve the performance of catalytic applications, and controlling the valence state of Cu to 1^+ is the key to successful synthesis of $CuCrO_2$.

The glycine nitrate process has been successfully employed to prepare nanosized, porous, stoichiometric, homogeneous $CuCrO_2$ and $CuFeO_2$ powders without ambient control. The as-prepared powders were nanosized into a spherical shape and crystallized in a delafossite structure. The powders showed a very large surface area compared to the powder synthesized by traditional method. These powders have potential to be applied as photocatalyst and Cu-base steam reforming catalyst.

100 nm 3D Laue Diffraction Technique for Ultra-High Spatial and Strain Resolution Combined with Versatile Analytical Probes for Materials Science

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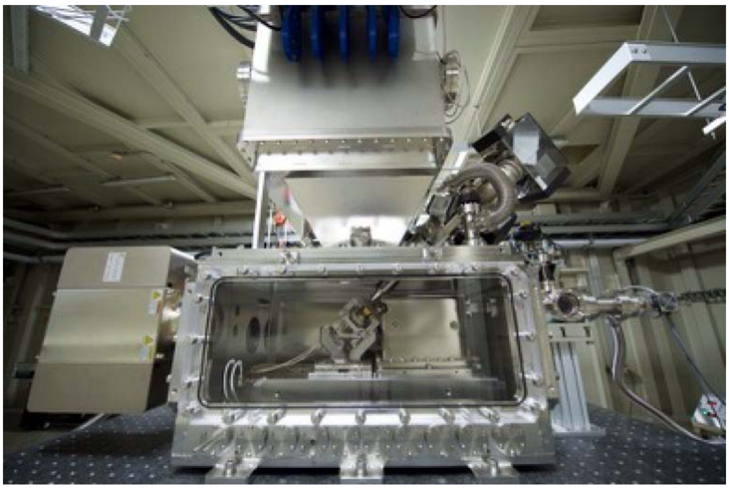
The X-ray Nanodiffraction Beamline (XND) is one of the phase-I projects for Taiwan Photon Source (TPS). Construction of the XND will complete before March of 2016 and commissioning for optics and end-station will follow. The end-station called "FORMOSA (FOcus x-Ray for MicrO-Structure Analysis)" is dedicated to use white/mono-beam Laue diffraction for structural analysis. For instance, users could obtain the 2D and 3D distribution of phases, orientation, residual strain, stress and dislocations for materials in a complex form without distorting the sample during measurement. The estimated spatial resolution could be better than 100x100x50 nm. Furthermore, this end-station provided many complementary tools. Quadro-probe stages collect optical, electrical, surface properties of specimens; the fluorescence detector provides elemental information and the cry-stage integrated with heater for temperature dependence experiments. Particularly, it is also the first time in synchrotron history to integrate an online scanning electron microscopy (SEM) as a navigator. With spatial resolution down to 4 nm, it is able to find out the interest region with tiny structure on samples and arrange the position for different probes. This end-station can function either in vacuum or ambient environments depending on the user's demands. In summary, XND beamline and FORMOSA end-station will provide not only 2D/3D-XRD but also XRF, XAS, XEOL/CL, SPM and SEM information for diverse research programs. The end-station is scheduled to open to user in early 2016.



Optical Properties and Exciton Dynamics of Organolead Halide Perovskite Nanocrystals

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In present study, we demonstrated that organolead bromide $CH_3NH_3PbBr_3$ perovskite nanocrystals (PNCs) with green photoluminescence (PL) have been synthesized by using a facile wet chemical method with aliphatic ammonium as capping ligands. The complete charge carrier dynamics of PNCs and the effects of capping ligands have been investigated by femtosecond transient absorption (TA) techniques and time-resolved photoluminescence (TRPL) spectroscopy. In addition, the $CH_3NH_3PbBr_3$ perovskite nanocrystals can be used as a matrix to tune the optical properties by varying the composition. The results indicate that the use of suitable capping ligand for PNCs can result in the interesting optical properties and are promising for potential applications including photovoltaics, detectors, and light emitting diodes (LEDs).

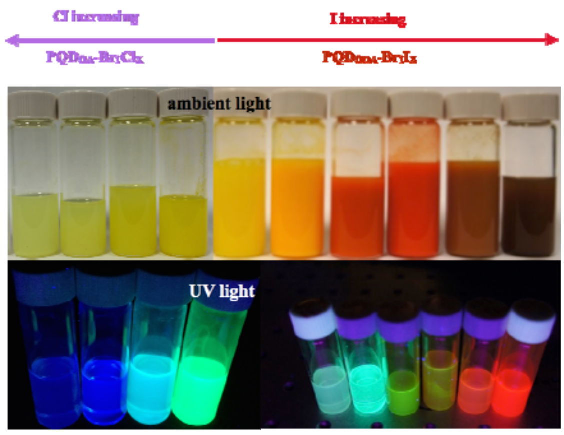

Figure 1. Tunable optical properties of mixed halide with $CH_3NH_3PbBr_3$ NCs as a matrix.

Synergistic Effect of Nitrogen and Sulfur Dual-Doped Non-precious Metal Catalysts for Oxygen Reduction Reaction

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This study discusses nitrogen and sulfur as the dual dopants in the iron-graphene catalysts (N-S-iron-graphene) for the oxygen reduction reaction (ORR) in fuel cells. After the pyrolysis in the optimized temperature, N-S-iron-graphene catalyst shows an excellent ORR activity and durability. The electron-transfer number is 3.99, which is very close to the ideal four electron-transfer number. In addition, the X-ray based techniques, such as X-ray diffraction (XRD), X-ray photoemission spectroscopy (XPS), and X-ray absorption spectroscopy (XAS) is used to analyze the relation between electronic structure and catalytic activity. In order to better understand the catalyst structure during the reaction, the *in-situ* technique is also utilized directly. It can elucidate the synergistic effects on the ORR activity and mechanism, which will provide understanding for future progress in the design of high activity non-precious metal catalysts.

XAS study of low dimensional dilute magnetic semiconductors

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Low Diluted magnetic semiconductors (DMSs), which possess the magnetic and semiconducting characteristics of materials, are promising candidates for developing the next-generation spintronics devices to use simultaneously the spin and charge characters of electrons. Electronically understanding the microscopic mechanism of mediating the magnetism of the DMS materials is of crucial importance to fabricate spintronics devices controllably through external fields like light and electric fields. The lecturer used X-ay absorption spectroscopy combining first-principles calculations explored the local atomic and electronic structures of numerous low-dimensional semiconductors, revealed the interplay of the dimension, structure and magnetism of magnetic semiconductors, illustrated the influence of the surface structure distortion on the bandgap structure of the semiconductors, and proposed a series of novel methods for tuning the magnetism of low-dimensional magnetic semiconductors via shell-core structure, phase doping, surface structure relaxation, valence alteration and so forth. All of these researches present themselves as a series of significant breakthrough in understanding the magnetic origin of magnetic semiconductors. The related results have been published in world-renowned journals like *J. Am. Chem. Soc.*, *Adv. Mater.*, *ACS Nano*., and *Appl. Phys. Lett.,* etc. To date, the applicant has published above 100 SCI articles which have been cited up to 1500 times by the peers, and undertook and accomplished 6 projects (including one key project) sponsored by Chinese National Science Foundation.

Capacitance of carbon based electrical double layer capacitors

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Supercapacitors store electrostatic energy in the electrical double-layer (EDL) at the interface between an electrode and an electrolyte and are key components in power source technologies. In order to fully realize their potential, the energy densities of these capacitors need to be increased. The structure features of the carbon materials, for example specific surface area (SSA), dopant and defect, are the key factors that dominate the EDL capacitance. We studied the dependence of the EDL capacitance on the SSA, dopant, and defect of carbon material by using a model electrode that was prepared by CVD-graphene sheets. The results show that the quantum capacitance suppress the EDL capacitance near the point of zero charge, and doping and defect improve the EDL capacitance by changing the quantum capacitance in a different way.

In-situ and on-time soft X-ray experiment: CO reduction by CuO electrocatalyst

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The trend to discuss the chemical energy storage and catalytic conversion becomes much important for the next generation of energy materials. Recently, the electrochemical reaction characterized by the active species and electric potential is conducted to the novel X-ray technology. Its probing consequence can provide the element-resolved and site-specific analysis to determine the chemical interaction at the interface. However, the solid-liquid interface and electrochemical environment are the tough problems to solve. An in-situ liquid cell with the vacuum seal by the thin X-ray window is established in the endstation of sort X-ray spectroscopy in the Taiwan light source. The measurement with in-situ environment and real-time control directly offers the understanding of the chemical and electronic structure information varied with the electrochemical redox interaction. In the present result, the chemical composition and bonded environment of the electrodeposited Cu on the Au surface are discussed for the correlation of oxygen evolution reaction under the electrochemical potential and molecule environment.

1	驚聲銅像廣場	Statue of Mr. Chang Ching-sheng	12	會文館(F)	Hwei-wen Hall (F)	22	文錙音樂廳	Carrie Chang Music Hall
2	大門警衛站	Main Entrance Guard House	13	商管大樓(B)	Business and Management Building (B)	23	學人宿舍	Faculty Residences
3	紹謨紀念游泳館(N)	Shao-mo Memorial Natatorium Complex (N)	14	海事博物館(M) 黑天鵝展示廳	Maritime Museum (M) Black Swan Exhibition Hall	24	覺生紀念圖書館(U)	Chueh-sheng Memorial Library (U)
4	騮先紀念科學館(S)	Liu-hsien Memorial Science Hall (S)	15	工學館(G)	Engineering Building (G)	25	覺生綜合大樓(I)	Chueh-sheng Memorial Hall (I)
5	鍾靈化學館(C)	Chung-ling Chemistry Hall (C)	16	工學大樓(E)	Main Engineering Building (E)	25	覺生國際會議廳(10樓)	Chueh-sheng International Conference Hall (10th Fl.)
6	圖書館鍾靈分館	Chung-ling Library	17	教育學院(ED)	College of Education (ED)	26	學生活動中心(R)	Student Activity Center (R)
7	傳播館(Q)	Communication Hall (Q)	18	松濤館(Z)	Sung-tao Hall (Z)	27	教職員停車場	Faculty Parking Lot
8	傳播館(O)	Communication Hall (O)	19	文錙藝術中心	Carrie Chang Fine Arts Center	28	視聽教育館(V)	Audio-visual Education Building (V)
9	紹謨紀念體育館(SG)	Shao-mo Memorial Gymnasium (SG)	20	外國語文大樓(FL)	College of Foreign Languages and Literatures (FL)	29	行政大樓(A)	Administration Building (A)
10	麗澤國際學舍(J)	Reitaku International House (J)	21	驚聲紀念大樓(T)	Ching-sheng Memorial Hall (T)	30	宮燈教室(H)	Chinese Palace-style Classrooms (H)
11	文學館(L)	College of Liberal Arts (L)	21	驚聲國際會議廳(3樓)	Ching-sheng International Conference Hall (3rd Fl.)	31	覺軒花園	Chueh-hsuan Chinese Garden