### The Chinese University of Hong Kong Division of Materials Science and Engineering

## **Projects Offered in 2025-26**

No.	Project title	Degree	Offered by
1	Synthesis and characterization of crystals of correlated electron materials	MPhil	Prof. Swee Kuan Goh
2	Alkaline metal batteries	PhD	<u>Prof. Quan Li</u>
3	Synthesis and characterization of topological materials	PhD or MPhil	<u>Prof. Yufan Li</u>
4	Synchrotron based studies on organic/perovskite solar cells	MPhil or PhD	<u>Prof. Xinhui Lu</u>
5	Topics in plasmonics and metamaterials	MPhil or PhD	Prof. Daniel H. C. Ong
6	Plasmon-powered artificial nitrogen fixation	PhD	Prof. Jianfang Wang
7	Synthesis and structural analysis of quantum materials	PhD	Prof. Qisi Wang
8	Topics in computational biophysics	PhD or MPhil	Prof. Yi Wang
9	Active matter engineering	PhD or MPhil	<u>Prof. Yilin Wu</u>
10	Surface and interface studies of important thin films and nano-materials	PhD	<u>Prof. Junyi Zhu</u>

### Synthesis and characterization of crystals of correlated electron materials (MPhil) (Prof. S. K. Goh, ≡ skgoh@cuhk.edu.hk)

Motivated candidates with strong interest in the physics of correlated electron solids are invited to participate in our research programme. Our group frequently studies the some of the high quality crystals under extreme conditions to follow the fate of their constituent electrons, such as exotic behaviors in superconductors and magnetic materials [1-3]. We run a stateof-the-art cryogen-free dilution refrigerator equipped with high magnetic field, in which several types of high pressure devices can be integrated. The successful candidate(s) will assist in the preparation and/or characterization of these crystals for indepth studies in our laboratory. Highly motivated students with a strong background of experimental solid state physics/solid state chemistry/material science are invited to apply. The applicants will be encouraged to work as a team because since collaborations among our department and international collaborators will be involved in their project. [One to two students may be admitted.]

### References:

- K. T. Lai, A. Takemori, S. Miyasaka, F. Engetsu, H. Mukuda, and S. Tajima, "Evolution of the phase diagram of LaFeP<sub>1-x</sub>As<sub>x</sub>O<sub>1-y</sub>F<sub>y</sub> (y=0-0.1)", Phys. Rev. B 90, 064504 (2014).
- K. T. Lai, P. Adler, Y. Prots, Z. Hu, C.-Y. Kuo, T.-W. Pi and M. Valldor, "Successive Phase Transitions in Fe<sup>2+</sup> Ladder Compounds Sr<sub>2</sub>Fe<sub>3</sub>Ch<sub>2</sub>O<sub>3</sub> (Ch = S, Se)", Inorg. Chem. 56, 12606 (2017).
- Y. J. Hu, Y. T. Chan, K. T. Lai, K. O. Ho, X. Guo, H.-P. Sun, K. Y. Yip, D. H. L. Ng, H. Z. Lu, and S. K. Goh, "Angular dependence of the upper critical field in the high-pressure 1T' phase of MoTe<sub>2</sub>", Phys. Rev. Mater. 3, 034201 (2019).

### 2. Alkaline metal batteries (PhD) (Prof. Q. Li, 🖃 liquan@cuhk.edu.hk)

This project works on materials and technology development for alkaline metal batteries, targeting at the next generation battery technology of high energy density and long cycle stability, such as solid state batteries and Li-metal batteries. There are two focus of the project: (i) Material (electrode, electrolyte, separator) design to achive high energy density, high rate performance, and long cycle life of the respective battery systems. (ii) mechanistic study to identify the evolution of the battery materials during charge/discharge cycles and improve their cycling performance. Up to two students may be admitted.

### **References** :

- 1. Hu XT, Gao Y, Sun YM, Hou Z, Luo YF, Wang DN, Wang JP, Zhang B, Zheng ZJ, Li Q, "Preserving the Li {110} texture to achieve long cycle life in Li metal electrode at high rates", Advanced Functional Materials, 202307404, 2023.
- 2. Hu XT, Gao Y, Zhang B, Shi L, Li Q, "Superior cycle performance of Li metal electrode with {110} surface texturing", EcoMat, e12264, 2022.

### Synthesis and characterization of topological materials (PhD or MPhil) (Prof. Y. F. Li, <u>yufanli@cuhk.edu.hk</u>)

Topological materials give rise to various exotic magnetotransport responses that show promising applications in cutting-edge computing, memory and sensing devices. In this project, we focus on (1) synthesizing thin films of topological material, (2) characterization of their magnetic and electrical transport properties, and (3) exploring potential applications related to giant anomalous/spin Hall effect and pure spin current phenomenon. Students with strong background in solid state physics are encouraged to apply. [One to two students may be admitted.]

### **References** :

- Y. Li, Q. Ma, S. X. Huang, C. L. Chien, "Thin films of topological Kondo insulator candidate SmB6: strong spinorbit torque without exclusive surface conduction", Science Advances 4, eaap8294 (2018).
- T. Liu, Y. Li, L. Gu, J. Ding, H. Chang, P. A. Praveen Janantha, B. Kalinikos, V. Novosad, A. Hoffmann, R. Wu, C. L. Chien, M. Wu, "Nontrivial nature and penetration depth of topological surface states in SmB6 thin films", Phys. Rev. Lett. 120, 207206 (2018).
- T. Higo, Y. Li, K. Kondou, D. Qu, M. Ikhlas, R. Uesugi, D.Nishio-Hamane, C. L. Chien, Y. Otani, S. Nakatsuji, "Omnidirectional Control of Large Electrical Output in a Topological Antiferromagnet", Adv. Funct. Mater. 2008971 (2021).

# 4. Synchrotron based studies on organic/perovskite solar cells (MPhil or PhD)

(Prof. X. H. Lu, 🖃 xinhui.lu@cuhk.edu.hk)

Nowadays, solar industry becomes the fastest growing industry due to the rising demands to solve energy crisis and environmental problems. Among various types of solar cells, organic photovoltaic devices offers low-cost, light weight and flexible solar energy harvesting, have attracted a lot of research effors. Recently, organic and inorganic halide perovskite solar cell has emerged as a rising star in the solar industry due to its astonishing progress in power conversion efficiency. This project focuses at using state-of-art synchrotron radiation technique to characterize the molecular and nano-scale structure information of this two types of thin film solar cell, understanding its correlation with device performance and in turn improving the power conversion efficiency of solar cells. [Two students may be admitted.]

#### **References** :

- 1. L. Dou, J. You, Z. Hong, Z. Xu, G. Li, R.A. Street and Y. Yang, "25th anniversary article: A decade of organic/polymeric photovoltaic research", Advanced Materials, (2013).
- 2. Kojima, K. Teshima, Y. Shirai and T. Miyasaka, "Organometal halide perovskites as visible-light sensitizers for photovoltaic cells", Journal of the American Chemical Society, 131 (2009) 6050-6051.
- J. Mai, T. K. Lau, J. Li, S. Peng, C. Hsu, U. Jeng, J. Zeng, N. Zhao, X. Xiao and X. Lu, "Understanding morphology compatibility for high-performance ternary organic solar cells", Chem. Mater, DOI: 10.1021/acs.chemmater.6b02264, (2016).

# 5. Topics in plasmonics and metamaterials (MPhil or PhD) (Prof. D. H. C. Ong, ≡ hcong@phy.cuhk.edu.hk)

Recently, plasmonics and metamaterial have both be named as a new eras after photonics and electronics. They serve as an important platform for studying the fundamentals of light matter interaction by manipulating the electromagnetic waves in an unconventional manner. Their applications include making high efficient light emitting diodes (LEDs) and solar cells, ultrahigh sensitive biosensors, passive and active optical elements for photonic circuitry, optical tweezers, etc. Our group focuses on two projects. The first one studies the interaction between plasmonic systems/metamaterials and quantum dots [1]. We engineer the near-fields around the quantum dots and study how their absorption and emission properties are affected. In particular, we measure the local density of the optical states around one single quantum dot in frequency, momentum, time, and space domains by using several home-built, specially designed microscopes. Its spontaneous emission rate, chirality, photocurrent generation efficiency, etc, are then studied accordingly so that LEDs and solar cells can be implemented eventually. The second project combines plasmonic tweezers and surface enhanced Raman scattering (SERS)/surface plasmon resonance (SPR) sensing in attempt to image single molecules. In principle, this combination produces an analogy of "line of sight" method by placing the target molecules at the right position where they can be seen easily. However, since both the manipulation and the sensing require the precision at the length scale of nanometers, a full knowledge of designing the plasmonic/metamaterial systems to yield suitable hotspots for biosensing, building appropriate characterization tools, generating strong optical force for grabbing the molecules, etc, is essential [2]. These two projects involve extensive collaboration with the theoretical group in Hong Kong University of Science and Technology. [Up to two students may be admitted.]

### **References** :

- M. S. Tame et al, "Quantum plasmonics", Nat. Phys. 9, 329 (2013); Z. L. Cao and H. C. Ong, "Determination of coupling rate of light emitter to surface plasmon polaritons supported on nanohole array", Appl. Phys. Lett. 102, 241109 (2013).
- 2. M. L. Juan et al, "Plasmon nano-optical tweezers", Nat. Photonics 5, 349 (2011); C. Y. Chan et al, "Dependence of surface enhanced Raman scattering (SERS) from twodimensional metallic arrays on hole size", Appl. Phys. Lett. 96, 033014 (2010).

### 6. Plasmon-powered artificial nitrogen fixation (PhD) (Prof. J. F. Wang, 🖃 *jfwang@phy.cuhk.edu.hk*)

Nitrogen is an essential ingredient in proteins and nucleotides. Although the atmosphere contains a large amount of nitrogen, most organisms cannot directly use nitrogen. Nitrogen needs to be fixed into ammonia or nitrate for use. The current industrial nitrogen fixation process consumes a lot of energy and produces a lot of carbon dioxide emissions. The realization of artificial nitrogen fixation in an environmentally friendly manner has become an important goal. Plasmonic nanoparticles can focus light extremely tightly. Their resonance wavelengths can be varied widely. Moreover, plasmon excitation can generate hot electrons and holes, which provides a new way for the photo-generation of hot charge carriers. Plasmonic nanoparticles can therefore overcome many disadvantages that are associated with traditional semiconductors for photocatalysis. We are intensively developing plasmonic photocatalysts for efficient artificial photocatalytic nitrogen fixation. Plasmonic nanoparticles are typically made of noble metals. We will focus on non-noble metal-based plasmonic nanomaterials. We will try to gain deep understanding about the working mechanism of our plasmonic photocatalysts and to achieve significant improvement in efficiency. We will also design flat-bed reactors that are suitable for large-area sunlight-driven nitrogen fixation. The project will involve nanomaterials synthesis, characterization, optical measurements, and photocatalytic tests. The project will require backgrounds and/or interests on nanomaterials and chemistry. Applicants who are interested in this topic are very welcome to join us. [Up to two postgraduate students will be admitted.]

# 7. Synthesis and structural analysis of quantum materials (PhD) (Prof. Qisi Wang, E qwang@cuhk.edu.hk)

This project will focus on the discovery of new quantum materials including high-temperature superconductors, quantum magnets, unconventional charge ordering systems, and other correlated materials. Detailed structural analysis based on x-ray diffraction measurements will be performed as an essential input to understand the novel physical properties. Motivated students with background of crystal growth and/or structural analysis using diffraction measurements are encouraged to apply. [Up to two students may be admitted.]

### 8. Topics in computational biophysics (PhD or MPhil) (Prof. Y. Wang, 🖃 <u>yiwang@cuhk.edu.hk</u>)

Computer modelling has become increasingly important in our understanding of the bioligcal world. Our research involves developing and applying computational methods to investigate the structure, function and dynamics of biological macromolecules, such as proteins, DNAs, and lipids. With the help of computers, we can model the motion of individual atoms of these macromolecules and then extract useful information from such motion using principles of statistical mechanics. A major area of our current work is the energetics and kinetics at the (nano)material-cell interface, where we combine modeling approaches at different spatial and temporal resolutions to examine, for example, how easy it is for a given nanoparticle to 'break' a lipid membrane [1], what enables a certain hydrogel to achieve underwater adhesion [2], and how fast a cell may spread in a 3D hydrogel [3]. The main approachs used in our group are molecular dynamics and free energy calculation techniques. Students interested in computer modeling related to biophysics are encouraged to apply. No biology background is required. [1 to 2 PhD or MPhil students may be admitted.]

### **References** :

- 1. Y. T. Pang, Z. Ge, B. Zhang, P. Xiu, Q. Li, Y. Wang, "Pore formation induced by nanoparticles binding to a lipid membrane". Nanoscale 12(14), 7902-7913, 2020.
- X. Peng, Y. Li, T. Li, Y. Li, Y. Deng, X. Xie, Y. Wang, G. Li, L. Bian, "Coacervate-derived hydrogel with effective water repulsion and robust underwater bioadhesion promotes wound healing", Advanced Science 9, 2203890, 2022.
- M. B. Yang, K. Wei, C. Loebel, K. Zhang, Q. Feng, R. Li, D. S-h Wong, X. Xu, C. Lau, X. Chen, P. Zhao, C. Yin, J. A. Burdick, Y. Wang, L. Bian, "Enhanced mechanosensing of cells in synthetic 3D matrix with controlled biophysical dynamics", Nature Communications 12:3514, 2021.

### 9. Active matter engineering (PhD or MPhil) (Prof. Y. L. Wu, 🖃 <u>ylwu@cuhk.edu.hk</u>)

Active matter is a fast growing, interdisciplinary field focusing on systems where energy is spent locally to produce mechanical work. This includes all living systems and synthetic self-driven materials. In this project we aim to elucidate the principles that govern active matter selforganization and self-assembly, and to understand how the emergent phenomena in active matter systems may give rise to novel mechanical functionalities. The results can be applied to fabricate autonomous and intelligent materials with life-like properties, setting the foundation for next-generation soft robotics, adaptive materials, and biomedical therapeutics. Our research is mainly driven by experiments, with the help of modeling, computer simulations and artificial Intelligence tools. We fuse experimental techniques from physics, chemistry and other disciplines to address different questions. Students with either experimental or theoretical background are welcome to apply. Knowledge in any one of the following subjects is preferred (but NOT required): statistical physics, continuum mechanics, optics, microscopy, chemical/biological engineering, physical chemistry, molecular biology, electrical engineering, and digital image processing. [One or two students may be admitted.]

### References :

- 1. To learn more about our current research please visit our lab website: <u>http://www.phy.cuhk.edu.hk/ylwu/index.html</u>.
- 2. Haoran Xu & Yilin Wu (2024) Self-enhanced mobility enables vortex pattern formation in living matter. Nature, 627, 553-558.
- 3. F. Ji, Y. Wu, M. Pumera, L. Zhang (2023) Collective behaviors of active matter learning from natural taxes across scales. Adv. Mater. 35, 2203959.
- 4. Haoran Xu, Mehrana R. Nejad, Julia M. Yeomans, Yilin Wu (2023) Geometrical control of interface patterning underlies active matter invasion. PNAS, 120 (30) e2219708120
- 5. Haoran Xu, Yulu Huang, Rui Zhang, Yilin Wu (2023) Autonomous waves and global motion modes in living active solids. Nature Physics, 19, 46-51.
- 6. Liu, S., Shankar, S., Marchetti, M. C., & Wu, Y. (2021) Viscoelastic control of spatiotemporal order in bacterial active matter. Nature, 590, 80-84.

### Surface and interface studies of important thin films and nano-materials (PhD) (Prof. J. Y. Zhu, <u>si jyzhu@phy.cuhk.edu.hk</u>)

"The Surface is the Devil's work." Surface can be considered as a two dimensional defect of a perfect crystal. Reactions, important physical and chemical processes often happen on surface. Surface has a profound effect on many material physical problems. Tuning surface properties can be critical in thin film growth and device properties. Many famous surface science problems have been solved using density functional theory (DFT) calculations. Applying DFT calculations and classic molecular dynamics calculations can be effective to study surface phenomena. Our goals are: investigating the surface reconstructions, surface passivation, surface diffusion, surfactant effects, surface effects on doping in many different thin films and nano-materials, including CZTS, InGaN, CIGS, AlGaP, diamond, SiC, ScTiO<sub>3</sub>, various topological insulators and super conductors. With deep understanding of the surface phenomena, it will be possible to reveal hidden physics mechanisms of important surface physics problems and enhance thin film or nano-materials performance. [One student may be admitted.]

### **References** :

- 1. J. Y. Zhu, F. Liu and G. B. Stringfellow, "Dual-surfactant effect to enhance p-type doping in III-V semiconductor thin films", Physical Review Letters, 101(19), 196103 (2008).
- Y. Zhang, K. He, C.-Z. Chang, C.-L. Song, et. al., "Crossover of the three-dimensional topological insulator Bi<sub>2</sub>Se<sub>3</sub> to the two-dimensional limit", Nature Physics 6, 584-588 (2010).
- 3. Y. Yan, R. Noufi and M. M. Al-Jassim, "Grain-boundary physics in polycrystalline CuInSe<sub>2</sub> revisited: experiment and theory", Phys. Rev. Lett. 96, 205501 (2006).