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

Projects Offered in 2020-21

No.	Project title	Degree	Offered by
1	Synthesis and characterization of high purity single crystals	MPhil	Prof. Swee Kuan Goh
2	Topics in cancer nanovaccine	PhD	Prof. Quan Li
3	Developing battery materials beyond Li-ion technology	PhD	
4	Synchrotron based studies on organic/perovskite solar cells	MPhil or PhD	Prof. Xinhui Lu
5	Topics in plasmonics and metamaterials	MPhil or PhD	Prof. Daniel H. C. Ong
6	Plasmonic driving of chemical reactions	PhD	Prof. Jianfang Wang
7	Topics in computational biophysics	PhD or MPhil	Prof. Yi Wang
8	Biomaterial self-organization and self-assembly	PhD or MPhil	Prof. Yilin Wu
9	Study of magnetotaxis of magnetotactic bacteria	MPhil or PhD	Prof. Ke-Qing Xia
10	Surface and interface studies of important thin films and nano-materials	PhD	Prof. Junyi Zhu

1. Synthesis and characterization of high purity single crystals (MPhil)

(Prof. S. K. Goh, *skgoh@phy.cuhk.edu.hk*,
http://www.phy.cuhk.edu.hk/skgoh/)

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 purest single crystals under extreme conditions to follow the fate of their constituent electrons. We run a state-of-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 single crystals for in-depth studies in our laboratory.

2. Topics in cancer nanovaccine (PhD)

(Prof. Q. Li, *liquan@phy.cuhk.edu.hk*,
http://www.phy.cuhk.edu.hk/qli/)

Nanoparticles serve as unique carriers for drugs, enabling controlled drug release and improved drug efficacy. In this project, we are interested in developing functionalized nanoparticulate systems as a general platform for applications in vaccine development, in particular, cancer vaccine. We aim at using our non-viral mRNA delivery system based on our in-house developed hybrid nanoparticle technology, to simultaneously deliver tumor antigen and a comprehensive set of molecular adjuvants, and evaluate the tumor-reactive immune response. Upto one student may be admitted.

***References* :**

1. *Fan L, Zhang SL, Zhang CY, Yin C, Song C, Lin G and Li Q, "Multidrug resistance in cancer circumvented using a cytosolic drug reservoir", Advanced Science, DOI: 10.1002/advs. 201700289, 2018.*
2. *Lena M. Kranz1 et al., "Systemic RNA delivery to dendritic cells exploits antiviral defence for cancer immunotherapy", Nature, 2016, doi:10.1038.*

3. Developing battery materials beyond Li-ion technology (PhD)

(Prof. Q. Li, *liquan@phy.cuhk.edu.hk*,
http://www.phy.cuhk.edu.hk/qli/)

This project works on materials development for batteries beyond the current Li-ion technology, such as sodium ion batteries and Li-S batteries. The project involves electrode material design, synthesis with composition and morphology control, various characterizations of the battery materials, and the performance measurement of the cells. There are two focus of the project: (i) Material/architectural 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. State-of-the-art characterizations including in operando XRD and in situ TEM studies will be carried out. Up to two students may be admitted.

***References* :**

1. *D. Lan et al., "Phase pure Sn4P3 nanotops by solution-liquid-solid growth for anode application in sodium ion batteries", Journal of Material Chemistry A, 2017, DOI: 10.1039/C6TA10685D.*
2. *Y. Huang et al., "Revisiting the origin of cycling enhanced capacity of Fe3O4based nanostructured electrode for lithium ion batteries", Nano Energy, doi.org/10.1016/j.nanoen.2017.10.001 .*
3. *D. Lan, et al.,"Cu4SnP10 as a promising anode material for sodium ion batteries", Nano Energy, 39, 506-512, 2017.*
4. *Liu H, et al., "High energy density aqueous Li-Ion flow capacitor", Advanced Energy Materials, DOI: 10.1002/aenm.201601248, 2016.*

4. **Synchrotron based studies on organic/perovskite solar cells (MPhil or PhD)**
(Prof. X. H. Lu, 🖃 *xhlu@phy.cuhk.edu.hk*,
🌐 *http://app.phy.cuhk.edu.hk/xhlu/*)

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.*
3. *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*,
🌐 *http://www.phy.cuhk.edu.hk/people/ong.html*)

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 :

1. *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 two-dimensional metallic arrays on hole size", Appl. Phys. Lett. 96, 033014 (2010).*

6. **Plasmonic driving of chemical reactions (PhD)**
(Prof. J. F. Wang, 🖃 *jfwang@phy.cuhk.edu.hk*,
🌐 *http://www.phy.cuhk.edu.hk/~jfwang/*)

Plasmonic nanomaterials possess strong localized plasmon resonances. Their light-absorption capabilities are strongly enhanced upon resonant excitation. Moreover, plasmon excitation can generate abundant hot electrons/holes, which can be used to drive a variety of chemical reactions for chemical synthesis as well as the conversion of solar energy into chemical fuels. In my group, we are devoted to the design of pure and hybrid nanostructures based on metals, oxides and semiconductors. Such nanostructures can effectively adsorb and activate reactant molecule, swiftly generate hot charge carriers, and efficiently convert light to heat. We will focus on the understanding of photon absorption, charge carrier generation and transport, charge carrier-induced chemical reactions as well as the improvement of the overall performances. Two types of applications will be targeted. One is the use of sunlight to drive the production of chemical fuels, such as water splitting, nitrogen fixation, and the other is the use of sunlight to drive many important catalytic chemical reactions for chemical synthesis. The project will involve nanomaterials preparation, characterization, simple optical measurements, and chemical reactions. [Two postgraduate students will be admitted.]

7. **Topics in computational biophysics (PhD or MPhil)**
(Prof. Y. Wang, 🖃 *yiwang@phy.cuhk.edu.hk*,
🌐 *http://www.phy.cuhk.edu.hk/yiwang/*)

Computer modelling is becoming increasingly important in our understanding of the bioligcal world. Our research is focused on developing and applying computational methods to investigate the structure, function and dynamics of biological macromolecules, such as proteins, lipids, and carbohydrates, etc. 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 [1-3]. Current work in our group revolves around biomembranes, which consist of lipid bilayers and embedded membrane proteins. Our research includes, for instance, how small molecules get through a membrane, how nanoparticles interact with a lipid bilayer, and how structure and dynamics of a membrane are affected by its lipid components, etc. Answers to the above questions will enable us to better understand drug permeability, design safer and more efficient nanoparticle drug carriers/biosensors, as well as elucidate a variety of membrane physical-chemical properties.

The main approachs used in our group are molecular dynamics and various free energy calculation techniques. While focus is placed on the application of these approaches, we also have a number of method development projects. Students interested in computer modeling of biomolecules are encouraged to apply. Some programming experiences are preferred but not required. No biology background is required. [1 to 2 PhD or MPhil students may be admitted.]

References **:**

1. *Y. Wang and J. A. McCammon. Introduction to molecular dynamics: theory and applications in biomolecular modeling. In N. V. Dokholyan, editor, Computational Modeling of Biological Systems: From Molecules to Pathways, Ch. 1, pp. 3-30, Springer-Verlag, 2012.*
2. *M. Karplus and J. A. McCammon. Molecular dynamics simulations of biomolecules. Nature Structural & Molecular Biology 9, 646-652, 2002.*
3. *M. Karplus. Nobel lecture: Development of Multiscale Models for Complex Chemical Systems: From H+H2 to Biomolecules, 2013. http://www.nobelprize.org.*

8. Biomaterial self-organization and self-assembly (PhD or MPhil)

(Prof. Y. L. Wu, 🖃 *ylwu@phy.cuhk.edu.hk*,
🌐 *http://www.phy.cuhk.edu.hk/ylwu/index.html***)**

Life is the most fascinating state of matter. The research in our lab lies at the interface of physics, biology, and material sciences: We seek to understand how living materials function, adapt and evolve.

Our current research aims to elucidate the principles that govern biomaterial self-organization and self-assembly. Knowledge learned from our studies may find applications in tissue engineering and in fabricating new bio-inspired devices or self-assembled materials. The study may also inspire new strategies to control the self-organization of "active matter". As a fast-growing and interdisciplinary field, active matter science studies systems composed of units where energy is spent to produce motion. This includes all living organisms, the subcellular constituents driven by molecular motors, and synthetic materials resulting from the self-organization of active elements. Students with background in biology, chemistry, soft matter, or engineering are welcome to apply. Knowledge in molecular biology, chemical/biological engineering, microscopy, electrical engineering, or digital image processing is preferred (but NOT required). [One or two students may be admitted.]

References **:**

1. *To learn more about our current research please visit our lab website: http://www.phy.cuhk.edu.hk/ylwu/index.html*
2. *C. Chen, S. Liu, X. Q. Shi, H. Chaté and Y. L. Wu, "Weak synchronization and large-scale collective oscillation in dense bacterial suspensions", Nature 542: 210-214 (2017).*
3. *"The physics of life", Nature 529, 16-18 (2016). doi:10.1038/529016a.*

9. Study of magnetotaxis of magnetotactic bacteria (MPhil or PhD)

(Prof. K. Q. Xia, 🖃 *kxia@phy.cuhk.edu.hk*,
🌐 *http://www.phy.cuhk.edu.hk/turbulence/***)**

Magnetotactic bacteria (MB) are microorganisms that contain magnetic crystals 30-50 nm in size. These crystals are enclosed by a lipid bilayer membrane and are called magnetosomes, which are usually formed in chain structures inside the cell. It is generally believed that MBs use their magnetosomes to align with the local magnetic field and move along the magnetic field lines. Such a behavior is referred to as magnetotaxis (or magneto-aerotaxis). An important issue in the studies of MB is whether the magnetotaxis is passive or active. In the former case, the magnetic field only aligns the MBs and their motion are driven by the oxygen gradients. This presumably simplified their search for favorable oxygen environment in aquatic habitat. In the latter case, MBs are thought to possess magnetic receptors similar to chemotaxis. In this project, student will carry out experiments that are designed to address the issue of whether the magnetotaxis of MBs are passive or active. [One student may be admitted.]

References :

1. *Arash Komeili, "Molecular mechanisms of magnetosome formation", Annu. Rev. Biochem. 76, 351 (2007).*
2. *Christian Jogler and Dirk Schuler, "Genomics, genetics, and cell biology of magnetosome formation", Annu. Rev. Microbiol. 63, 501 (2009).*
3. *Nadège Philippe and Long-Fei Wu, "An MCP-like protein interacts with the MamK cytoskeleton and is involved in magnetotaxis in magnetospirillum magneticum AMB-1", J. Mol. Biol. 400, 309 (2010).*

10. Surface and interface studies of important thin films and nano-materials (PhD)

(Prof. J. Y. Zhu, 🖃 *jyzhu@phy.cuhk.edu.hk*,
🌐 *http://www.phy.cuhk.edu.hk/people/zhu.html***)**

"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, $ScTiO_3$, 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).*
2. *Y. Zhang, K. He, C.-Z. Chang, C.-L. Song, et. al., "Crossover of the three-dimensional topological insulator* Bi_2Se_3 *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 $CuInSe_2$ revisited: experiment and theory", Phys. Rev. Lett. 96, 205501 (2006).*