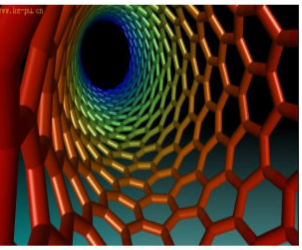
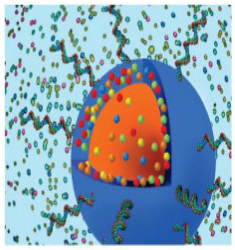
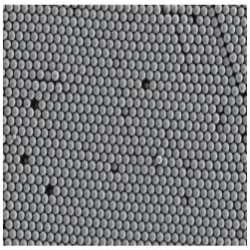
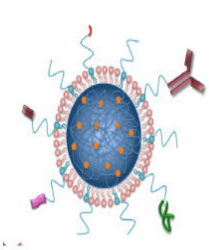
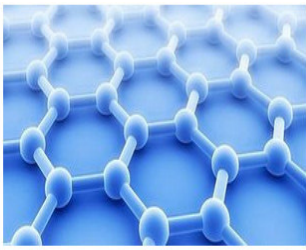
QUT-SEU Workshop on Nano Biotechnology



Workshop Handbook

Organizers:

Science and Technology Institute, Southeast University

School of Biological Science & Medical Engineering, Southeast University

July 10th-July 13th, 2013, Nanjing, China

Content

Scientific Program

July 11th (Thursday)

Shaw Science and Technology Museum Hall

9:00-9:30	Opening Ceremony (Minqiang Hu, Jianqing Li, John Bell) Chairperson: Ning Gu
Oral Presentation (25min+5min)	Chairperson: YuanTong Gu
9:30-10:00	**John Bell** Engineering Thin Film Semiconductor Gas Sensors
10:00-10:30	**Songqin Liu** Nano-bio-probe for Imaging and Therangostics of Cancer Cells
10:30-11:00	**Zhiyong Li** Identifying Vulnerable Atherosclerotic Plaque: Insights from MRI and Biomechanics
Coffee Break (10min)	
Oral Presentation (25min+5min)	Chairperson: Songqin Liu
11:10-11:40	**YuanTong Gu** Advanced meshfree methods and multiscale techniques in computational engineering and science
11:40-12:10	**Yu Zhang** High-performance Magnetic Nanoparticles and Their Application in MR Imaging and Hyperthermia Therapy
Lunch	
Oral Presentation (25min+5min)	Chairperson: John Bell
13:40-14:10	**Suvash Saha** Computational Fluid Dynamics (CFD) and its applications
14:10-14:40	**Yuanjin Zhao** Photonic Crystal Encoded Microbeads for Multiplex Bioassays
14:40-15:10	**Haifei Zhan** MD simulations to explore the mechanical deformation mechanisms of perfect and defected nanowires
15:10-15:40	**Xin Zhou** A Novel Strategy for Detecting Pathogen
Coffee Break (10min)	
Oral Presentation (25min+5min or 12min+3min)	Chairperson: Xin Zhou

15:50-16:20	**Fang Yang** Magnetic Microbubbles and Their Application for Ultrasound and Magnetic-resonance Dual Modality Imaging
16:20-16:35	**Tong Li** A novel hierarchical multiscale model for microfilament networks
16:35-16:50	**Cuiping Yang** Novel targeted therapy of multiple myeloma CSCs by anti- ABCG2 monoclonal antibody combined with Paclitaxel- Fe3O4 NPs
16:50-17:05	**Xubo Lin** Probe the Interactions of Nanoparticles with the DPPC Monolayer using MD Simulations
Dinner	

Abstracts

Oral-1

Engineering Thin Film Semiconductor Gas Sensors

John Bell
School of Chemistry, Physics and Mechanical Engineering, Queensland University

Thin film semiconductor gas sensors typically operate at temperatures above 400°C, but lower temperature operation is highly desirable, especially for remote area field sensing as this reduces significantly power consumption. We have investigated a range of sensor materials based on both pure and doped tungsten oxide (mainly focussing on Fe-doping), deposited using both thermal evaporation and electron-beam evaporation, and using a variety of post-deposition annealing. The films show good sensitivity at operating temperatures as low as 150°C for detection of NO_2. There is a definite relationship between the sensitivity and the crystallinity and nanostructure obtained through the deposition and heat treatment processes, as well as variations in the conductivity caused both by doping and heat treatment. The ultimate goal of this work is to control the sensing properties, including selectivity to specific gases through the engineering of the electronic properties and the nanostructure of the films.
In addition, the research strengths and excellent research environment in QUT especially in School of Chemistry, Physics and Mechanical Engineering will be also introduced.

Oral-2

Nano-bio-probe for Imaging and Therangostics of Cancer Cells

Songqin Liu
School of Chemistry and Chemical Engineering, Southeast University

MicroRNAs (miR) have played key cancer biomarkers that regulate tumor suppressor genes. Hence, simultaneous detecting and inhibiting of miR function will be useful as a cancer theragnostics probe to minimize side effects and invasiveness. We developed a cancer-targeting therangostics probe in a single nano-system using an AS1411 aptamer and miR-21 molecular beacon (miR-21 MB) conjugated fluorescence silica nanoparticle (FSNAS miR-21 MB) to simultaneously target to cancer cell, image intracellularly expressed miR-21 and treat miR-21 involved carcinogenesis. The nano-system displayed a great selectivity and delivery into a human breast cancer MCF-7 cell line. The miR-21 MB detached from the FANAS miR-21 MB in the cytoplasm of MCF-7 cells imaged miR-21 biogenesis. Importantly, there was no emission cross-talk between the MB and fluorescence silica nanoparticle, thereby ensuring accurate detection of intracellular miR-21. Simultaneously MB resulted in antitumor therapeutic effects by inhibiting miR-21 function, indicating a successful theragnostics. FANAS miR-21 MB can be easily applied to other cancers by simply changing a targeted miR highly expressed in cancers cells.

Oral-3

Identifying Vulnerable Atherosclerotic Plaque: Insights from MRI and Biomechanics

Zhi-Yong Li
School of Biological Science and Medical Engineering, Southeast University

Plaque rupture is responsible for the majority of myocardial infarction or ischaemic stroke in the developed world. Available screening and diagnostic methods are insufficient to identify the victims before the event occurs. Non-invasive methods to identify additional new and emerging biomarkers to assess plaque vulnerability and predict possible rupture before the fatal event actually happens are urgently called for. In vivo MRI-based computational models for atherosclerotic plaques were developed to perform mechanical analysis to quantify critical flow and stress/strain conditions related to plaque rupture which often leads directly to heart attack or stroke. A combination of in vivo high resolution MRI and biomechanical analysis could potentially act as a useful tool to assess plaque vulnerability and risk stratify patients with carotid atheroma. Further investigations are needed in: high resolution imaging, atheroma mechanical property assessment, multi-scale modelling, computational methods and model validation. Multi-modality interdisciplinary approach may lead to more complete data, new discoveries, and possible clinical applications.

Oral-4

Advanced meshfree methods and multiscale techniques in computational engineering and science

YuanTong Gu
School of Chemistry, Physics and Mechanical Engineering at Queensland University

Multiscale characterization has been a recent focus in the development of advanced technology, and has posed new challenges, because the length/time scales to be analyzed vary from macroscopic to nanoscopic dimensions and many analytical tools are only applicable to a single dimensional scale. This research aims to develop a concurrent simulation technique, based on the combination of the meshfree method (MM) and the molecular dynamics (MD), for analyzing the deformation of systems that need the integration of material properties from nanoscopic to macroscopic dimensional scales. The developments and research outcomes of the advanced meshfree/meshless methods are firstly reviewed and discussed, and then the multiscale MM/MD modeling technique is developed. In addition, the major researches are undertaking in Prof. Gu' s group, including computational bio-mechanics, computational nanostructures and numerical modelling for industry applications, will be also introduced.

Oral-5

High-performance Magnetic Nanoparticles and Their Application in MR Imaging and Hyperthermia Therapy

Yu Zhang
School of Biological Science and Medical Engineering, Southeast University

Magnetic nanoparticles have exhibited a wide range of biomedicine applications, including magnetic resonance imaging (MRI), triggered drug release and magnetic fluid hyperthermia. The fabrication of high-performance magnetic nanoparticles with controllable size, morphology, composition and aggregation can further improve their magnetic properties and enhance MRI contrast and magnetically induced heating efficiency, as well as significantly decrease injection dose and toxic and side effect. In this study, monodisperse magnetic ferrite nanoparticles with

various size and morphologies, including 0-D spherical, cubical and starlike nanocrystals and 3-D nanoclusters, have been successfully synthesized via high-temperature decomposition of metal acetylacetonate (acac) in the presence of oleic acid (OA) and oleyamine (OAm). Our studies also reveal the transformation process of 0-D nanocrystals to 3-D nanoclusters as well as the formation mechanism, which provide a versatile synthetic strategy for shape-controlled nanoparticles. These nanoparticles have the high magnetization, MRI relaxivity and magnetically-induced heating in an alternating current magnetic field, which have successfully employed as passive targeting MRI contrast agents and heating agents for diagnosis and treatment of breast cancer on a mouse model when PEGylated using DSPE-PEG2000.

Oral-6

Computational Fluid Dynamics (CFD) and its applications

Suvash Saha
School of Chemistry, Physics and Mechanical Engineering at Queensland University

Computational Fluid Dynamics is a strong tool in fluid mechanics that numerically analyzes the fluid flow, heat and mass transfer. This CFD calculation involves solving partial differential equations such as Navier‐Stokes and energy equations with appropriate boundary conditions. Since these equations are highly nonlinear, it is almost impossible to get the analytic solutions. However, it is possible to get some analytic solutions based on different stages of the flow development where dominant terms of the equations can be equated. This is called scaling analysis where those approximate results are correct to one order of magnitude. This presentation will cover scaling analysis of boundary layer due to different thermal forcing applied on different types of geometries. Validation of scaling analysis will also be discussed. At the end, several applications of CFD simulations will be shown in this presentation.

Oral-7

Photonic Crystal Encoded Microbeads for Multiplex Bioassays

Yuanjin Zhao
School of Biological Science and Medical Engineering, Southeast University

Multiplex assays have attracted considerable interest to meet the growing demand for clinical diagnosis, gene expression, drug discovery, and so on. Most of the assays are based on molecular binding or recognition events. In this point, different probe biomolecules could be immobilized to encoded carriers, which can be mixed and subjected to an assay simultaneously and then many binding events can be distinguished by their codes. Herein we summarize our work on self-assembled photonic beads as novel encoded carriers of biomolecules in multiplex bioassays. We have successfully fabricated different kinds of encoded photonic beads with controlled size and monodispersity by microfluidic device. The beads with opal structure and inverse opal structure could be used in multiplex labeling detection and label-free detection of biomolecules, respectively. These photonic beads provide a new coding strategy of suspension array for low cost, sensitive and simultaneous multiplex bioassay.

Oral-8

MD simulations to explore the mechanical deformation mechanisms of perfect and defected nanowires

Haifei Zhan
School of Chemistry, Physics and Mechanical Engineering at Queensland University

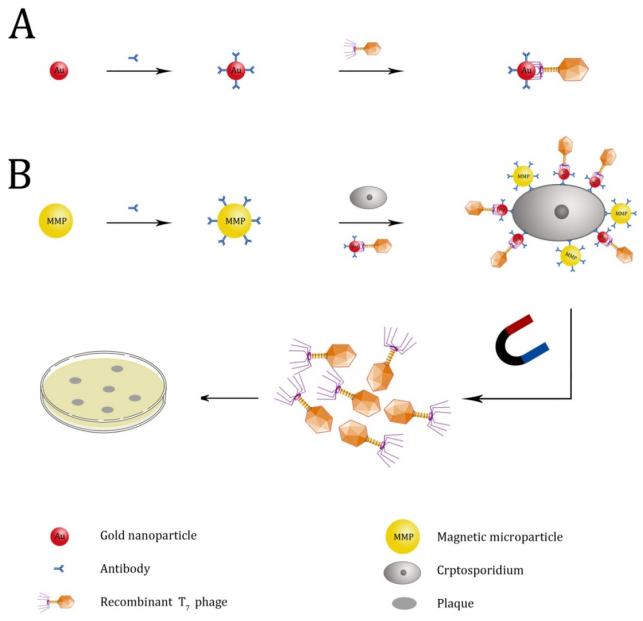
Nanowires (NWs) have attracted appealing and broad applications owing to their remarkable mechanical, optical, electrical, thermal and other properties. To unlock the revolutionary characteristics of NWs, a considerable body of experimental and theoretical work has been conducted. However, due to the extremely small dimensions of NWs, the application and manipulation of the in situ experiments involve inherent complexities and huge challenges. For the same reason, the presence of defects appears as one of the most dominant factors in determining their properties. Using large-scale molecular dynamics (MD) simulations, the mechanical properties and deformation mechanisms of different NWs under diverse loading conditions including tension, compression, bending, vibration and torsion are accessed. These nanowires include different FCC metal NWs (e.g., Cu, Ag, Au NWs) and Si NWs, which are either in a perfect crystal structure or constructed with different defects (e.g. Pre-existing surface/internal defects, grain/twin boundaries, and stacking faults). This study greatly extends and enhances the existing knowledge and understanding of the properties/performance of NWs, and will eventually benefit the realization of NWs' full potential applications.

Oral-9

A Novel Strategy for Detecting Pathogen

Xin Zhou
School of Biological Science and Medical Engineering, Southeast University

The project aims to develop an absolute quantification strategy for detecting pathogen. The proposed method is based on magnetic microparticle (MMP) probes and gold nanoparticle (GNP) probes modified with an engineered fluorescent T7 phage. The key objective will be to detect the presence of a few pathogens in water in less than 4 hours. This will enable rapid detection of 'outbreaks' which occur in Chinese urban environments and can cause significant gastro illnesses and health hazard.



Schematic of the Novel strategy

Oral-10

Magnetic Microbubbles and Their Application for Ultrasound and Magnetic-resonance Dual Modality Imaging

Fang Yang
School of Biological Science and Medical Engineering, Southeast University

With the development of micro- and nano- delivery carrier, in recent years, many researches have shown that both microbubbles (MBs) and magnetic nanoparticles (MNPs) individually can be demonstrated great promise as effective imaging contrast agents and drug delivery carriers. Combination of the above-mentioned dual-phase character, magnetic microbubble formulations have been developed as novel approach for delivery systems, analytical biochemistry and in vitro/ vivo theranostics. Such MBs can combine the advantages of the individual carriers and overcomes many of their limitations. Herein we summarize our work on the fabrication of magnetic microbubble structure and their application in medical imaging and treatment. The basic physical characteristics and behaviour of magnetic and nonmagnetic microbubbles indicate that the high echogenicity is not reduced by the decorating of magnetic nanoparticles. Thus, the magnetic microbubbles with the desired shell flexibility can be visualised by using ultrasound imaging, magnetic resonance imaging. And they can also be localized using an externally applied magnetic or acoustic field for therapeutic delivery.

Oral-11

A novel hierarchical multiscale model for microfilament networks

Tong Li
School of Chemistry, Physics and Mechanical Engineering at Queensland University

F-actin is polymerized from G-actin in living cells, and performs as the structural basis for the mechanical performance and dynamic behaviors of microfilament networks. The molecular mechanisms of force generation and transference on actin filament networks are crucial to the understandings of mechanobiology of cellular processes in living cells. At sub-nanoscale, we have employed quantum chemistry calculation to understand the biophysics in F-actin dynamics. A hierarchical multiscale model for microfilament networks was developed at nano/microscale to investigate the mechanical stabilization of actin related cell dynamics. The interaction between actin and graphene is also studied by all atom molecular dynamics simulation to understand the biocompability of 2D carbon material in biomedical applications. We have also conducted experimental studies of mechanical testing on single living cells and cartilage. The extended knowledge of the biomechanics of living cells and tissues can help understand the biological behaviors of living organisms and further serve the design and manufacturing of artificial biomaterials in surgical replacement.

Oral-12

Novel targeted therapy of multiple myeloma CSCs by anti- ABCG2 monoclonal antibody combined with Paclitaxel- Fe3O4 NPs

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Multiple myeloma (MM) is a malignant plasma cell disorder that results in skeletal lesions, renal insufficiency, hypercalcemia or anemia, which still remains incurable. The purpose of this study was to investigate the targeting therapeutic effects of anti-ABCG2 monoclonal antibody (McAb) combined with paclitaxel-Fe_3O_4 nanoparticles (PTX-NPs) on $CD138^-CD34^-$MM cancer stem-like cells (MM CSCs) isolated from human MM cell line RPMI 8266 and patient samples by immune magnetic activated cell sorting method. Non obese diabetic/severe combined immunodeficiency mice were intravenously injected with MM CSCs and treated with NPs, McAb, melphalan in combination with predisone (MP), PTX, PTX-NPs or McAb combined with PTX-NPs (McAb-PTX-NPs), respectively. McAb-PTX-NP led to a significant alleviation in the bone and renal lesions in contrast to using a single agent detected by Micro-Computer tomography scanning and ultrasonography. The targeted therapeutic efficacy mechanism may be related to inducing MM CSC apoptosis. This is the first time to report the anti-MM CSC efficacy by McAb combined with PTX-NPs *in vivo*. The novel strategy may be more considered in order to obtain long-term remission in MM patients.
Keywords: Multiple myeloma; Cancer stem cells; ABCG2; Monoclonal antibody; Paclitaxel; Fe3O4; Nanoparticles

Oral-13

Probe the Interactions of Nanoparticles with the DPPC Monolayer using MD Simulations

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Molecular dynamics simulation is powerful tool in studying dynamic process of molecular system and shows its significance in assisting experiments to clarify certain molecular mechanism, which has been considered as a "Computational Microscope" for molecular biology[1]. Here, we use molecular dynamics simulation to probe the interactions between nanoparticles (NPs) and the DPPC monolayer (model pulmonary surfactant) based on the existing experimental results (such as Langmuir-Blodgett technique, AFM, etc.), which may provide insights for both promoting respiratory drug delivery using NPs as carriers and assessing the potential toxicity of exposed engineering NPs.

[1] Ron O. Dror, Robert M. Dirks, J.P. Grossman, HuafengXu, and David E. Shaw, "Biomolecular Simulation: A Computational Microscope for Molecular Biology," Annual Review of Biophysics, 2012, 41, 429-452

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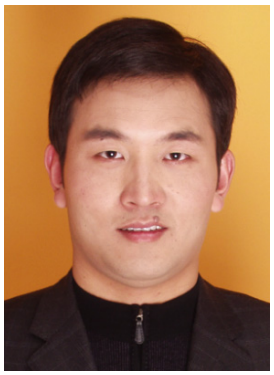

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