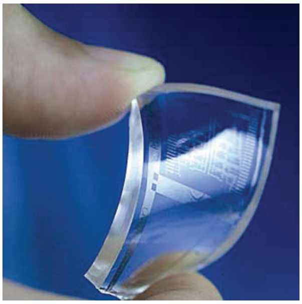
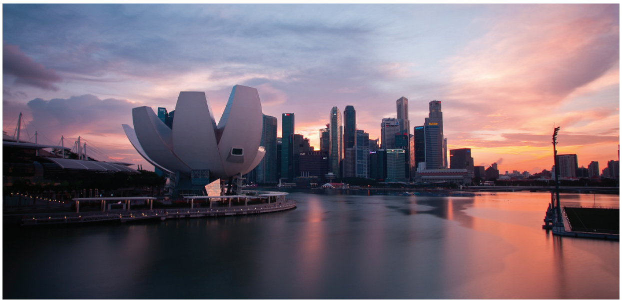
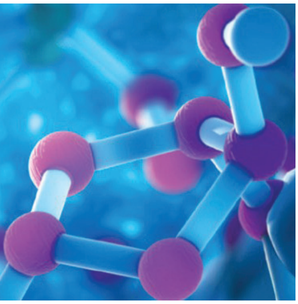
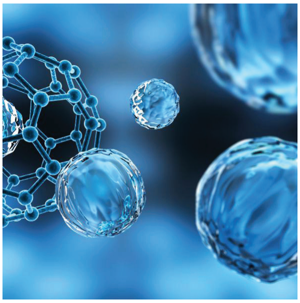
Accepted Abstracts

Smart Materials & Polymer Chemistry 2019



Joint event on

WORLD CONGRESS ON SMART MATERIALS AND STRUCTURES

&

3rd International Conference on

POLYMER CHEMISTRY AND MATERIALS ENGINEERING

November 21-22, 2019 | Singapore

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The fusion of material science, cyber-physical security and information science for next generation tools for treaty verification, safeguards and non-proliferation

David Mascarenas
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Arms controls treaties are vital for ensuring global security. A guiding principle for the development of these treaties is that they should be verifiable. Continuity-of-knowledge of the state of treaty-verifiable items must be maintained to ensure that they are not modified or swapped out in a manner inconsistent with the treaty. Verification of arms control treaties pose unique, multidisciplinary technical challenges. The challenges involve concerns related to cyber-physical security issues, maintaining knowledge barriers, distributed sensor networks, structural health monitoring, non-destructive evaluation, and sensing. It is often the case that treaty verification personnel only have limited time and physical access to treaty-accountable items. In many cases the treaty-accountable items spend the vast majority of the time under the control of parties that might have an interest in tampering with the treaty-accountable items. Current technologies for verifying treaties do not adequately address these challenges. This presentation will focus on the development of technologies that intimately combine material science with signal processing, machine learning, and cyber-physical security to candidate tools for the next generation of treaty verification. Specifically we fill focus on the development of a remotely readable, graphite-oxide tamper-evident seal and the potential for the use of the magnetic Barkhausen noise effect to establish unique fingerprints of nominally similar ferrous components. Both of these technologies combine material science with information science and security concepts. Undoubtedly other research opportunities exist for combining material science and information science to enable new technologies not only for treaty verification, but other commercial applications that require continuity-of-knowledge of the state of physical objects.

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Application of the discrete element modelling in air drying of particulate solids

Jintang Li[1] and **David J Mason**[2]

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The Discrete Element Method (DEM) has been widely used as a mathematical tool for the study of flow characteristics involving particulate solids. One distinct advantage of this fast-developing technique is the ability to compute trajectories of discrete particles. This provides the opportunity to evaluate the interactions between particle, fluid and boundary at the microscopic level using local gas parameters and properties, which is difficult to achieve using a continuum model. To date, most of these applications focus on the flow behaviour. This paper provides an overview of the application of DEM in gas-solids flow systems and discusses further development of this technique in the application of drying particulate solids. Several sub-models, including momentum, energy and mass transfer, have been evaluated to describe the various transport phenomena. A numerical model has been developed to calculate the heat transfer in a gas-solids pneumatic transport line. This implementation has shown advantages of this method over conventional continuum approaches. Future application of this technique in drying technology is possible but experimental validation is crucial.

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Algorithmically discovering high temperature superconductors with quantum computers

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Superconductors play an integral role in magnetic resonance imaging (MRI), nuclear magnetic resonance (NMR) and fusion reactors for magnetic confinement. When they were first discovered in the early 20th century, it was unclear what physics went behind making them work. Since then, we have come a long way in describing at least one class of superconductors: low temperature, Type I and Type II superconductors. The mechanism giving rise to this class of low temperature superconductors is quantum mechanical in nature. Therefore, it is conceivable that such processes can be modelled easier and with more robustness on quantum computers as opposed to classical computers. This modelling ability can then be exploited to explore a broader search space of other superconductors that may have not been discovered yet.

ReactiveQ has created a computational engineering platform that allows for multi-physics simulations to be run on classical supercomputers as well as quantum computers. In lieu of accelerating the discovery of new materials, namely superconductors, ReactiveQ looked at the viability of both near-term, Noisy Intermediate Scale Quantum (NISQ) algorithms as well as long-term Universal Gate model algorithms that could be used to automate the discovery of high temperature superconductors.

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Preparation & pyroelectric properties evaluation of lead lanthanum zirconate itanate (PLZT) for waste heat power generation

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The combination of novel electrothermodynamic cycle based on temporal temperature variations and the pyroelectric effect is one of the potential method for utilizing the waste heat energy as a renewable energy source.

Lanthanum-modified lead zirconate titanate (PLZT) ceramics with concentration of La (5-7%), are located at and near the phase boundary between the rhombohedral and tetragonal ferroelectric phases at room temperature, which shows that these ceramics are possible as the candidates for a further improvement of power generating performance. In this study, we propose the relaxor ferroelectric ceramic x-mol% La- modified Lead Zirconate Titanate, PLZT x/65/35 (x= 6, 7, 7.5) which is known for having a good squareness of hysteresis loop and high dielectric constant. The power generating potential is evaluated theoretically by using hysteresis loop and measurement, and experimentally by using the DSW circuit to convert waste heat to practical energy.

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Sodium alginate/polyethyleneimine hydrogel: An effective material for the adsorption of heavy metal ions in water and catalysis

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Water pollution created by heavy metal ions becomes worldwide concern because of indiscriminate disposal of industrial wastewater in pure water system. In this work, we report a natural and highly efficient sodium alginate (ALG)/polyethyleneimine (PEI) composite hydrogel fabricated by a chemical crosslinking method for the removal of heavy metal ions from wastewater. The adsorption of heavy metal ions was thoroughly investigated in single ion adsorption and multi ions adsorption systems. In addition, after the adsorption we in situ reduced the Cu+2 ions forming a Cu NPs-loaded hydrogel, which proved an excellent catalyst as evidenced by the reduction reaction of 4- nitrophenol. We believe that the as-prepared ALG/PEI hydrogel will present an effective and practical paradigm for the cascaded treatment and recycling of heavy metal ions in wastewater.

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The use of piezoelectric based monitoring techniques in monitoring of curing process

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The unique transduction capability of piezoelectric materials allow them to be employed as active sensors for the purpose of structural health monitoring (SHM). Early development of these piezoelectric based monitoring techniques, such as the electromechanical impedance (EMI) technique and the wave propagation (WP) technique, mainly focus on their ability in monitoring damage of engineering structures. Their application have later been extended to monitoring of curing process of certain civil engineering materials. This is particularly useful for materials such as concrete and structural adhesive, which require considerable time for stiffness and strength development. Recent studies show that the use of piezoelectric based monitoring techniques could potentially replace the conventional destructive based testing techniques. Real time and remote monitoring is also possible. This study provides a comprehensive review of recent development of the piezoelectric based monitoring techniques in this particular application.

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Reaction kinetics in chemical engineering

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In the lecture is presented a theoretical analysis of the role of the reaction kinetics in chemical engineering for the solution of the main problems in the chemical industry (biotechnology, heat energy), i.e. the optimal design of new devices and the optimal control of active processes. The thermodynamic and hydrodynamic approximations for the modeling of the industrial process rates are presented and analyzed.

The industrial processes are the result of reactions, i.e. creation or disappearance of a substance and (or) heat as a result of chemical and (or) physical processes and their rate is determined by the reaction kinetics.

The reactions deviate the systems from the thermodynamic equilibrium and as a result processes arise, who are trying to restore that equilibrium. The rate of these processes can be determined by Onsager's "linearity principle", where the rate of the process depends linearly on the deviation from the thermodynamic equilibrium.

The Onsager's linearity coefficient can be determined after solving the hydrodynamics, mass transfer and heat transfer equations, where it is proportional to the mass transfer (heat transfer) coefficient.

The relations between the Onsager's linearity coefficient and mass transfer coefficient are presented for different processes.

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Drug delivery systems based on PCL nanoparticles obtained by non-aqueous emulsion polymerization

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Cancer remains one of the world's most devastating diseases responsible for more than 20% of all deaths. The conventional cancer treatments are generally associated with a series of toxic side effects: cytotoxicity, neurotoxicity, nephrotoxicity. In order to minimize these drawbacks, the achievement of reliable and efficient delivery systems of therapeutics, by the means of nanotechnology, is highly recommended.

Drug delivery systems can play a key role in the fight against cancers by delivering locally the anticancer drugs, and the efficiency of this delivery depends on several factors, such as: drug bioavailability, drug absorption processes, pharmacokinetic processes, timing for optimal drug delivery. The nanoparticles (NPs) are based on biocompatible polymers and their advantages are high drug encapsulation efficiency; improved drug bioavailability; solubility and retention time; enhanced chemical and biological stability; controlled drug release rate; wide variety of administration routes.

New controlled drug delivery systems based on poly(Ɛ-caprolactone) (PCL) biocompatible NPs were prepared by a non-aqueous emulsion polymerization starting from CL-in-PDMS non-aqueous emulsions stabilized with tailor-made PDMS-b-PCL block copolymers. In this type of emulsion, usually designated as oil-in-oil (o/o) emulsion, the monomer droplets are dispersed in a non-miscible oil and the stabilization can be achieved by using suitable block copolymers. After the polymerization reaction, the size of the obtained PCL particles, in the absence and in the presence of a model drug, was determined by DLS.

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