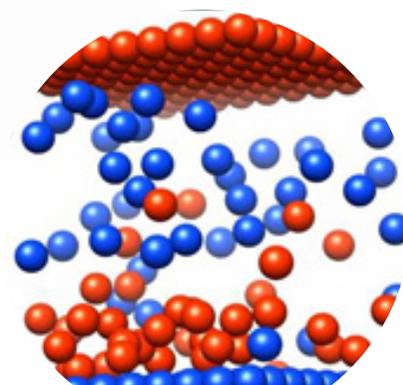
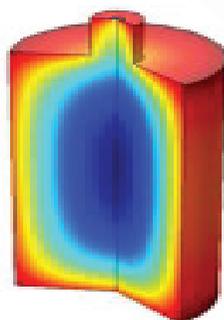
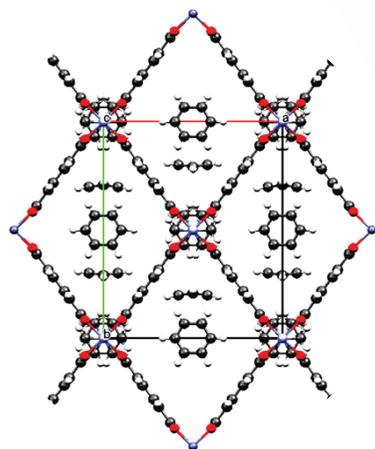
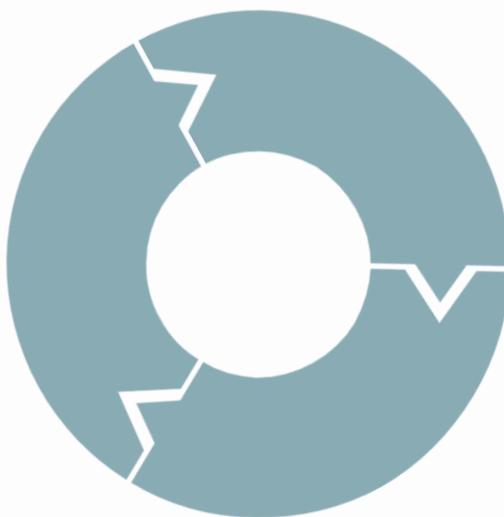
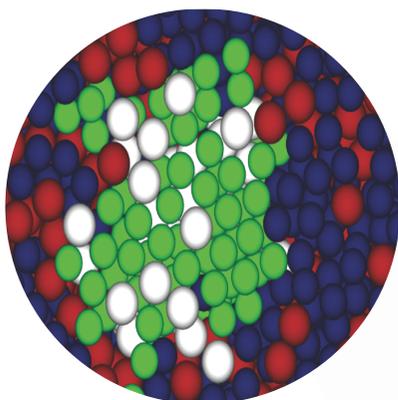
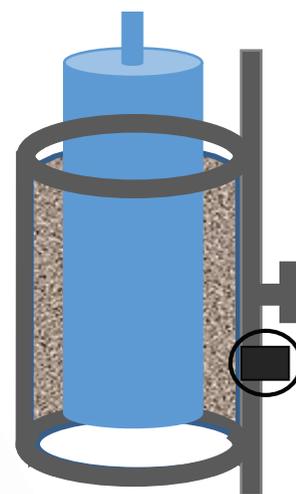
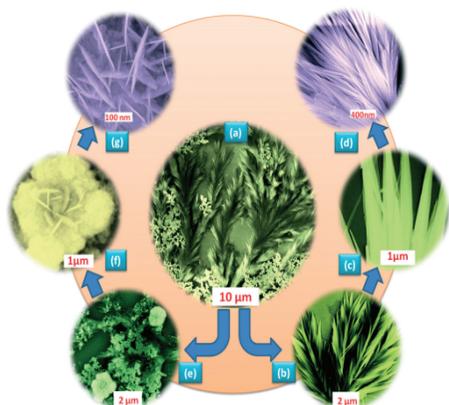


# ABSTRACT BOOKLET

2016



# **ChemE In-House Symposium (CIS) 2016**

**February 13, 2016**



**Department of Chemical Engineering**

**Indian Institute of Science (IISc), Bangalore**



**WELCOME**



## Technical Programme

<b>08:30 – 08:45</b>	<b>Registration &amp; Coffee</b>	
<b>08:45 – 08:55</b>	<b>Chairman's address</b>	
08:55 – 09:50	C.C. Lakshmanan, Chief scientist, ITC	<b>Plenary talk:</b> Some insights in to translating R&D to commercialisation
<b>Session I</b>		
09:50 – 10:10	K. Kesava rao	The Gibbs-Tolman model for calculating the surface tension of pure liquids and binary liquid mixtures from equations of state
10:10 – 10:25	Krishnaraj K P	A dilation-driven vortex flow in sheared granular materials explains a rheometric anomaly
10:25 – 10:40	Jaju S J	Structure-rheology relationship in lamellar phases
<b>10:40 – 11:00</b>	<b>Coffee &amp; Photo session</b>	
<b>11:00– 12:00</b>	<b>Poster session I</b>	
<b>Session II</b>		
12:00 – 12:20	Sharad Sontakke, ICT Mumbai	Anodic materials for DSSC: synthesis and applications
12:20 – 12:35	Praveen Kumar B	Enhancement of nucleation of protein crystals on nano-wrinkled surfaces
12:35 – 12:50	Rajasekharan M	Water adsorption on graphene oxide
12:50 – 13:05	Pushkaraj Joshi	Low-cost paper-based plasmonic sensors
<b>13:05 – 14:00</b>	<b>Lunch</b>	
<b>Session III</b>		
14:00 – 14:20	Banani Chakraborty	Functional DNA-origami: In the crossroad of top down & bottom up nanotechnology
14:20 – 14:35	Rubesh R	Estimating the prevalence of drug resistant strains of hepatitis C virus
14:35 – 14:50	Jatin Panwar	Single cell RNA counting using droplet microfluidics
<b>14:50 – 15:50</b>	<b>Poster session II</b>	
<b>Session IV</b>		
15:50 – 16:05	Kshetramohan Sahoo	Spinning bowl spinning disc contactor: Mixing studies and synthesis of nanoparticles
16:05 – 16:20	Ravikiran M	Detailed kinetic models for CO oxidation and Water gas shift reaction over Noble metal ionic catalysts
16:20 – 16:35	Satyapaul Singh	Hydrogen generation and utilization techniques at low temperatures
16:35 – 16:50	Naga Samrat MVV	Modeling the adsorption of fluoride onto activated alumina
<b>16:50 – 17:00</b>	<b>Coffee</b>	
<b>Panel discussion</b>		
<b>17:00 – 17:50</b>	<b>Grand challenges for chemical engineers in 21<sup>st</sup> Century</b>	
<b>17:50 – 17:55</b>	<b>Prizes</b>	
<b>17:55 – 18:00</b>	<b>Vote of thanks</b>	

## Poster Session I

P 1	Surya Narayana Murthy	Lattice Boltzmann for elastic solids
P 2	Ganesh Madabattula	Mathematical modeling of self-discharge in electrochemical capacitors
P 3	Aritra Santra	DSMC Simulation of high mach number turbulent flow in channel
P 4	Aslam Ansari MD	Alternative designs to harness natural convection in flow batteries
P 5	Disha Jain	Mechanistic and kinetic studies of CO oxidation over pristine and noble metal modified Fe <sub>2</sub> O <sub>3</sub> using DRIFTS
P 6	Satyaghosh Maurya	Investigating oligomerization pathways of ClyA pore forming toxin (PFT) on artificial bilayer membranes
P 7	Shivanand Kumar	Molecular simulation studies on gas hydrates
P 8	Tulsiram & Anusha	Detection of multiple targets via aptamer binding in solution and reporting with shape specific visual readout on DNA origami surface
P 9	Vadhana V	Phase transitions under nanoscale confinement: First order or second order?
P 10	Peter Varun D'souza	Secondary flow in slow granular flows in a Taylor- Couette viscometer
P 11	Kaushal Verma	Molecular simulation of Electric double layer Capacitor (EDLC)

## Poster Session II

P 12	Phanibhargava	The puzzle of Iridium nanoparticle synthesis
P 13	Ayush Agarwal	Interaction studies of pore forming toxins with supported lipid bilayer platforms
P 14	Phanikanth SVSSR	Motion of a spherical particle near a thin porous slab. An exact solution in bipolar coordinates
P 15	Ram Narayan C	Esterifying fatty acids with higher alcohols without using a catalyst
P 16	Rimzhim Gupta	Effect of morphology of Zinc oxide in ZnO/CdS/Ag ternary nanocomposite towards photocatalytic inactivation of <i>E.coli</i> under visible light
P 17	Archana C	Multifunctional C <sub>3</sub> N <sub>4</sub> / NiCo <sub>2</sub> O <sub>4</sub> composite for photocatalytic degradation
P 18	Saurabh Umrao	Characterizing DNA Aptamer based biosensors using single molecule spectroscopy
P 19	Yogesh Kailas B	Discrete element modeling to study mechanical behaviour analysis of human hair fibre
P 20	Anukrati Goel	Study of foam stability and bubble size using colloidal particles
P 21	Subbarao K	Dendrimers as nanoscale blocker for the toxic protein pores
P 22	Sushant kumar	Millifluidic reactor for room temperature synthesis of gold nanoparticles

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## The Gibbs-Tolman model for calculating the surface tension of pure liquids and binary liquid mixtures from equations of state

*Sukesh Tumram, Paul Mathais, S. Sundaresan, M.S. Ananth, and K. Kesava Rao*

Surface tension plays an important role in bubble and drop formation at low flow rates, peak heat flux in nucleate boiling, mass transfer from large bubbles, sprays of fuel droplets in combustors, and waves on falling liquid films. It also permits insects such as water striders to walk on water. The variation of the surface tension  $\sigma$  with the temperature can be described by empirical correlations, classical thermodynamics, or statistical thermodynamics. Gibbs developed the thermodynamics of a liquid-vapour system by introducing a dividing surface, which is a hypothetical surface that separates the system into two homogeneous phases. Correction terms are assigned to the dividing surface to account for the smooth variation of properties across the actual transition layer between the phases. Tolman (1948, 1949) considered a more detailed model of the interfacial region, and by comparing his equations with those of Gibbs, obtained expressions for  $\sigma$  and the location of the surface of tension. The latter is a particular dividing surface, chosen to simplify the analysis. Based on qualitative arguments, Tolman introduced a surface of discontinuity, such that the pressure  $p$  increases from its saturation value  $p_{\text{sat}}$  to a maximum value as the surface is approached from the vapour side, and  $p$  decreases from  $p_{\text{sat}}$  to its minimum value  $p_{\text{min}}$  as the surface is approached from the liquid side. By assuming an exponential decay of  $p$  away from the surface, Tolman obtained an explicit expression for  $\sigma$  in terms of  $p_{\text{sat}}$ ,  $p_{\text{max}}$ ,  $p_{\text{min}}$ , and two length scales  $\lambda_l$  and  $\lambda_v$ , where the subscripts  $l$  and  $v$  denote liquid and vapour, respectively. In the present work, Tolman's model is used along with the equations of state of van der Waals (1873) and the Lee and Kesler (1975) to fit data for 159 pure liquids, with an absolute average deviation (AAD) of 3.7 % and 1.8 %, respectively. For 56 binary mixtures, the AAD was 2.9 % for the Lee and Kesler equation of state. Even though the agreement is fairly good, the parameter  $\lambda_v$  turns out to be negative. While the reason for this behaviour is not clear, the Gibbs-Tolman model is aesthetically appealing and is a simple model that provides a route for predicting a surface property from a bulk equation of state.

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**Notes:**

## **A dilation-driven vortex flow in sheared granular materials explains a rheometric anomaly**

*Krishnaraj K.P. and Prabhu R. Nott*

Granular flows occur widely in nature and industry, yet a continuum description that captures their important features is yet not at hand. Recent experiments on granular materials sheared in a cylindrical Couette device revealed a puzzling anomaly, wherein all components of the stress rise nearly exponentially with depth. Here we show, using particle dynamics simulations and imaging experiments that the stress anomaly arises from a remarkable vortex flow. For the entire range of fill heights explored, we observe a single toroidal vortex that spans the entire Couette cell, and whose sense is opposite to the uppermost Taylor vortex in a fluid. We show that the vortex is driven by a combination of shear-induced dilation, a phenomenon that has no analog in fluids, and gravity flow. Dilatancy is an important feature of granular mechanics, but not adequately incorporated in existing models.

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**Notes:**

## Structure-rheology relation in lamellar phases

*S. J. Jaju and V. Kumaran*

Self-assembly of surfactant molecules at interface increases stability of oil-water mixtures. The micro-structures, thus formed, dictate the flow behaviour in such systems. In present work, we examine shear alignment of an initially disordered lamellar mesophase system. Lamellar phase, at equilibrium, is essentially a stack of surfactant bilayers. Such equilibrium state, however, is never achieved in practice due to defects and misaligned domains. We study structure-rheology relationship for lamellar fluid flow for a large parameter space. The scaling behaviour observed in simulations for excess viscosity and structural order parameters compares favourably with the analytical results.

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**Notes:**

## **Anodic materials for DSSC: Synthesis and applications**

*Sharad Sontakke*

*Department of chemical engineering, ICT Mumbai*

Titania ( $\text{TiO}_2$ ) is conventionally used as charge carried material in Dye Sensitized Solar Cells (DSSC). FTO or ITO coated glasses are the preferred anodic materials along with Titania. The efficiency of DSSC is shown to be a function of shape and properties of these anodic materials ( $\text{TiO}_2$  and ITO/FTO). In my research group, we synthesis; characterize; and explore various applications of titania as well as ITO. We have developed a method of fabricating ITO coated conducting glasses using synthesized materials. The research also focuses on synthesis of metal oxides of difference morphology (nanorods, flowers, nanospheres, nanowires, etc.) A DSSC fabricated using synthesized materials is found to be comparable (in terms of efficiency) with the one fabricated using commercial materials. However, the main advantage of using synthesized (or homemade) materials is the overall economy of the process. Various aspects related to the progress of ongoing research work will be discussed.

**Keywords:** DSSC, nanorods,  $\text{TiO}_2$  paste, ZnO flowers

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**Notes:**

## Enhancement of nucleation of protein crystals on nano-wrinkled surfaces

*Praveen Bommineni and Sudeep N. Punnathanam*

Synthesis of high quality protein crystals is essential for determining their structure. Hence development of strategies to facilitate nucleation of protein crystals is of prime importance. Recently, Ghatak and Ghatak[1,2] reported heterogeneous nucleation of protein crystals on nano-wrinkled surfaces. Through a series of experiments on different proteins, they were able to obtain high quality protein crystals even at low protein concentrations and sometimes without the addition of a precipitant. In this study, the mechanism of protein crystal nucleation on nano-wrinkled surfaces is studied through Monte Carlo simulations. The wrinkled surface is modeled by a sinusoidal surface. Free-energy barriers for heterogeneous crystal nucleation on flat and wrinkled surfaces are computed and compared. The study reveals that, the enhancement of nucleation is closely related to the two step nucleation process seen during protein crystallization. There is an enhancement of protein concentration near trough of the sinusoidal surface which aid in nucleation. However, the high curvature at the trough acts as a deterrent to crystal nucleus formation. Hence, significant lowering of the free-energy barrier is seen only if the increase in the protein concentration at the trough is very high.

### References:

1. A. S. Ghatak and A. Ghatak, Ind. Eng. Chem. Res., 2011, 50, 12984–12989.
2. A. S. Ghatak and A. Ghatak, Langmuir, 2013, 29, 4373–4380.

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### Notes:

## Water adsorption on graphene oxide

*Rajasekharan M and K. Ganapathy Ayappa*

Graphene oxides are graphene sheets with surface and edge carbon atoms having functional groups. The functional groups consist of epoxy, hydroxyl and carboxyl groups. As a consequence graphene oxides have hydrophilic and hydrophobic regions at the molecular level. Recently, it has been found that graphene oxide is a promising material for water desalination. Graphene oxide membranes have been found to exhibit higher water flux (4 - 10 times higher than current nanofiltration membranes). The GO membranes have also shown higher selectivity towards CO<sub>2</sub> even in humid conditions. The graphene oxide membranes show higher selectivity for hydrogen in H<sub>2</sub>/CO<sub>2</sub> and H<sub>2</sub>/N<sub>2</sub> mixtures. Hence they are promising materials for gas separations. Other applications of graphene oxides include printable electronics, solar cells, fuel cells and bio-sensors. In order to understand the high permeabilities reported for graphene oxide membranes in aqueous solutions, it is important to study the molecular interactions of water at the graphene oxide interface. Our study focuses on the adsorption of water on graphene oxides using grand canonical Monte Carlo simulations. We have carried out plane wave periodic density functional theory calculations to optimize the molecular structure of graphene oxide. The partial atomic charges are derived using ab-initio Hartree - Fock method and the atomic charges are obtained using CHELP-G scheme. These charges are used in classical Monte Carlo simulations. The optimized potential for liquid simulation (OPLS-AA) forcefield is employed in classical Monte Carlo simulations.

GCMC simulations reveal interesting water film growth as the vapor pressure is increased. Water is found to initially adsorb at the hydrophilic - hydrophobic interface. Subsequently water bridge spanning the hydrophilic region is observed. Hydrophobic/Hydrophilic ratio plays a key role in water layering and organization on the GO surface and adsorption isotherms. Separated water islands with increasing hydrophobicity is observed. Large number fluctuations are observed in graphene oxide due to the Janus nature of the interface.

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**Notes:**

## Low-cost paper-based plasmonic sensors

*Pushkaraj Joshi and V. Santhanam*

Low-cost, point of care diagnostic devices like wearable sensors, surface swabs for detecting hazardous chemicals is a rapidly growing field. Surface Enhanced Raman Spectroscopy (SERS) is an important technique for molecular analysis under ambient conditions, and the use of plasmonic nanostructures on paper as a disposable SERS substrate is an attractive option for low-cost, point-of-use analysis. Silver nanostructures are ideal candidates for use as SERS substrates, however, the activity of pre-fabricated silver nanostructures is affected by oxidation and necessitates either storage under inert gas conditions or a using a protective layer on the surface. Neither of these approaches are satisfactory in terms of cost and performance in real-world settings. Here, we report a print-expose-develop process, based on salt printing technique used in early silver-halide photography, to fabricate SERS active silver nanowire networks on demand using a desktop inkjet printer (~ 2000 INR). This process involves only the printing of silver and halide salt solutions and obviates the need for complex colloidal ink formulation steps used in literature reports on inkjet printed SERS substrates. The printed and photo-exposed silver halide films can be stored under ambient conditions and the latent silver can be easily developed into nanostructured silver at the point of use by dipping in a standard photographic developer solution. These silver nanostructures exhibit high (average EF ~  $2 \times 10^6$ ) and uniform ( $\sigma \sim 10\%$ ) SERS activity across the substrate. The act of storing silver in latent form within a silver halide film, effectively confers an unlimited shelf-life and can greatly reduce the cost of SERS substrates. The use of such paper-based SERS substrates to detect pesticide residues on the skin of fruits will also be highlighted.

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**Notes:**

## **Functional DNA-origami: in the crossroad of top down & bottom up nanotechnology**

*Banani Chakraborty*

DNA is a well-known biomolecule, which proved to have function in biology as well as in material world. Since 1982 DNA has been used widely to build nanostructures in 1D, 2D and 3D with very high precision and programmability in nanometer to micron scale. Since 2006 construction with DNA has become all the more easier with the introduction of DNA origami, where computer program is used to fold kilobases long viral genomic DNA in desired shape and size. Introduction of DNA origami merged the biology with material science by implementing long viral DNA as well as short chemically synthesized DNA or RNA to build the desired shapes in nano domain. Past decade has seen tremendous progress in complex structure formation with DNA origami in 2D and 3D. The power of bottom up nanotechnology is to form structures below 50nm with very high precision. Focus has been shifted in past few year from designing structures to making those functional for various applications. Having the flexibility to modify DNA chemically to perform desired functions on DNA origami as well as modifying DNA sequences specifically for host guest complexation (aptamer technology) is being studied to prepare the 1<sup>st</sup> DNA nano-biochip of its kind which will enable the detection of multiple targets in parallel in a 50 nm\*100 nm size chip. Individual sensors are tested with minute details using single molecule fluorescence in bulk as well as on surface. The limit of detection number of target is bound by the visualization technique detection limit; such as AFM, SEM. We are also focusing on forming hybrid nano-materials to enhance the precision and robustness of nanofabrication.

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**Notes:**

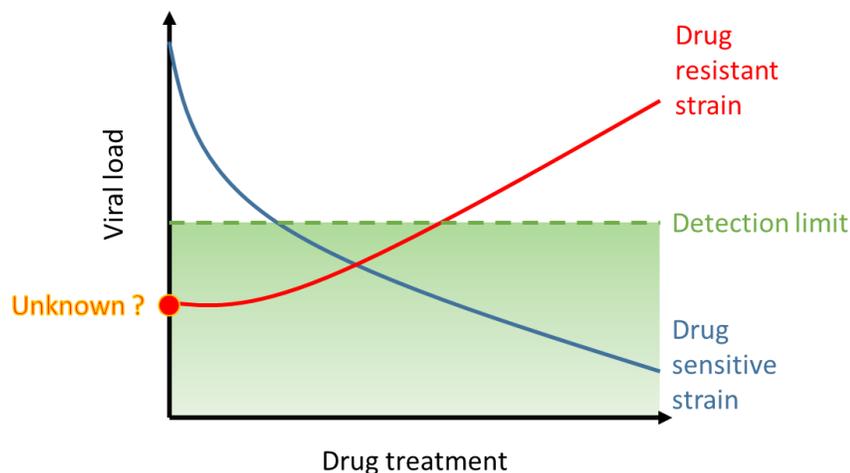
## *Estimating the prevalence of drug resistant strains of hepatitis C virus*

*Rubesh Raja, Aditya Pareek, Kapil Newar, Narendra M. Dixit*

HCV affects hepatocytes (liver cells) causing chronic infection. Currently, 170 million people in the world are chronically infected with HCV. DAAs, drugs targeting specific steps of HCV's lifecycle, are used in HCV treatment. The pre-existence of HCV genomes carrying mutations resistant to DAAs can compromise treatment outcomes. The frequencies of pre-existing resistant mutants are difficult to measure; current sequencing techniques cannot distinguish between rare mutants and sequencing errors. We developed a multi-scale mathematical model of HCV viral kinetics and evolution to estimate these frequencies.

We considered viral evolution at nucleotide positions where mutations contribute to resistance to a given DAA. We described viral replication in individual hepatocytes using fully stochastic dynamics and predicted the rates of mutant genome production from hepatocytes infected by different founder strains. We next considered a population of hepatocytes mimicking the liver and described this sequential accumulation of mutations by combining viral kinetics and evolution and predicted the steady-state frequencies of different mutants. We found that the frequencies depended on the genetic barrier of the drug, the underlying fitness landscape, and the mutational pathways involved.

We applied our model to several DAAs. We estimated the pre-treatment frequency of the mutant R155K, resistant to telaprevir, to be 0.019%, in close agreement with its frequency in the genotype 1 sequence database. We also estimated the pre-existing frequency of the daclatasvir resistant mutants Y93H/N/C/F to be 0.023%. Our model can be extended to other drugs, facilitating comparative evaluation of their susceptibility to resistance.



**Notes:**

## Single cell RNA counting using droplet microfluidics

Jatin Panwar, Raghavan Vardarajan<sup>1</sup>, Rahul Roy

<sup>1</sup>Molecular Biophysics Unit, IISc Bangalore.

Cell to cell heterogeneity plays a significant role in the underlying mechanisms of how individual cells process information and respond to perturbations. One such interesting example is isogenic populations of antibiotic-sensitive bacteria having rare cells that transiently become drug tolerant ‘persisters’<sup>1</sup>. Transcriptional profiling of isolated persisters has suggested a possible role of the TA (toxin-antitoxin) systems in persistence<sup>2</sup>. In bacteria, TA systems are found in both plasmids and chromosomes, but in most cases, their functional role is unclear, especially for genomic TA systems. We are examining the role of Ccd (control of cell death) TA system of *E.coli* which codes for an unstable antitoxin CcdA and a toxin CcdB. To understand the transcriptional regulation of CcdAB system and quantify it at single cell in a high throughput manner using microfluidics and fluorescence microscopy, we are developing a single cell RNA counting method using droplet microfluidics. Our integrated microfluidic device is designed to quantify the expression from the CcdAB operon using four distinct unit operations. First phase allows for the encapsulation of single cells into independent monodispersed aqueous picolitre droplets dispersed in an immiscible carrier oil using a microfluidic T-junction<sup>3</sup>. The droplet will contain lysis buffer and isothermal PCR amplification reagents along with probes tagged with fluorescent dyes to detect particular RNA of interest. The trapped cells in droplets are collected in a reservoir where they undergo lysis in their respective drops in the second phase. The third phase employs a flow focussing channel for breaking the primary drops into secondary droplets of the order of 10 femtolitres. The low concentration of RNA for most genes in single bacterial cells including CcdB ensures a Poisson distribution of molecules in the secondary droplets. The final phase includes a microchannel coupled with a Peltier heating device kept at 65°C where the RNA undergoes isothermal PCR amplification and fluorescence based ‘digital’ detection. By maintaining the order in the droplet flow, we can assign each secondary droplet to its parent primary drop and hence each RNA to its cell. This integrated microfluidic platform has a potential to bring high throughput single cell single molecule analysis as an easily employable tool to the fields of point of care diagnostic, proteomics, enzyme kinetics, reaction engineering and most essentially in biomedical research<sup>4</sup>.

**References:**

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**Notes:**

## **Spinning bowl spinning disc contactor: Mixing studies and synthesis of nanoparticles**

*Kshetramohan Sahoo and Sanjeev K. Gupta*

The creation of mono-disperse new solid phase through liquid phase precipitation route and synthesis of desired product through fast reactions calls for mixing of two liquids at molecular/micro scale without back-mixing. A process intensification device, named spinning disc spinning bowl (SBSD) contactor, developed earlier in our group, is expected to offer good micro-mixing without significant back-mixing at high processing rates. In a SBSB contactor, one liquid stream is fed to rotating bowl at the bottom, where from the liquid rises up in the form of a thin film as a result of centrifugal pressure differential. Droplets of the other liquid are spun off from the edge of a spinning disc, which impact the rising film on the bowl wall and get carried away to the collector at the top.

Here, we present findings of our studies on flow visualization, mixing characterization, and synthesis of drug and metal nanoparticles in a SDSB. We used a digital camera with controlled duration flash to freeze dynamic structures. The extent of micro-mixing is probed by using Iodide-iodate reaction. The absorbance due to the reaction product at 353 nm was used as primary indicator of mixing effectiveness. The synthesis of nanoparticles of drug Curcumin is carried out by using anti-solvent precipitation route and that of silver metal nanoparticles using reactive precipitation route.

## Detailed kinetic models for CO oxidation and Water gas shift reaction over Noble metal ionic catalysts

*Ravikiran M. and Giridhar Madras*

‘Noble metal ionic catalysts’ i.e. solid solutions of noble metals substituted in ionic state into base supports, have shown superior activity compared to their impregnated counterparts for gas phase reactions. This activity was attributed to the better dispersion of the metal on the supports, ionic state of the noble metals and creation of oxygen vacancies in case of reducible catalysts. In light of numerous experimental and spectroscopic studies for various gas phase reactions over these catalysts, detailed study covering the underlying surface chemistry of the gas phase reactions over these catalysts is still lacking. On the other hand, rigorous modeling procedures using DFT though offer a qualitative understanding, their ready applicability to gas phase reactions over reducible catalysts at atmospheric conditions is yet to be established.

Microkinetic modeling, which is detailed modeling procedure to elucidate reaction mechanisms of gas phase reactions over noble catalysts, can offer an intuitive understanding into the underlying surface chemistry of various gas phase reactions over reducible catalysts.

Among various gas phase reactions CO oxidation and Water Gas Shift reaction are prominent reactions in many industrial applications. In order to understand the reaction chemistry underlying these gas phase reactions detailed micro kinetic models were proposed. The validity of these models was tested over noble metal ionic catalysts, i.e. palladium doped ceria and platinum doped ceria was tested for CO oxidation and WGS reactions. From the results obtained, it was inferred that CO oxidation over palladium doped ceria proceeds via dual site mechanism and WGS over platinum proceeds via Redox mechanism. Furthermore, the rate expressions developed assuming appropriate rate determining steps for the presented mechanisms predicted the experimental observations even at higher temperatures this validating the robustness of the proposed microkinetic models.

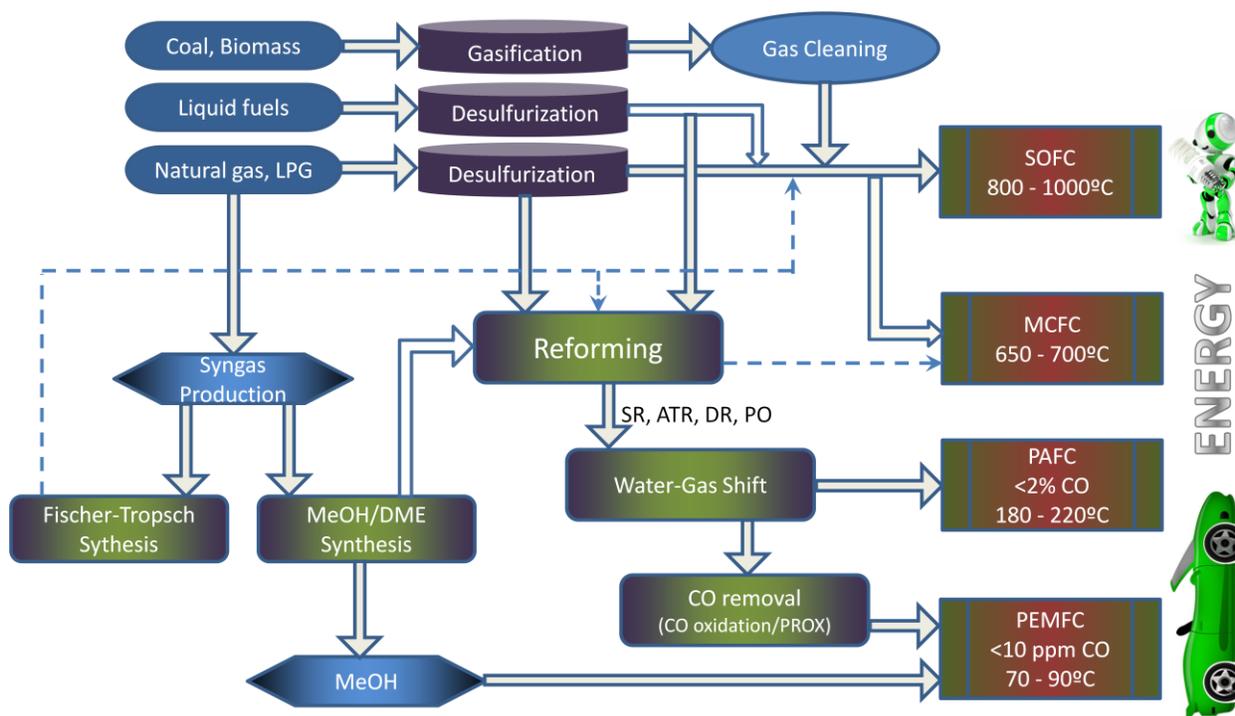
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**Notes:**

## Hydrogen generation and utilization processes at low temperatures

*Satyapaul A. Singh and Giridhar Madras*

Hydrogen is one of the renewable successors of fossil fuels due to its potential application in energy sector. Although it is 9<sup>th</sup> abundant material on Earth, industries are facing huge challenge to produce high purity hydrogen and hydrogen in form of syngas (CO and H<sub>2</sub> mixture). H<sub>2</sub> is being utilized for wide variety of applications like electricity generation using polymer electrolyte membrane fuel cell (PEMFC), rocket fuels, indoor heating, internal combustion, coolant and liquid fuels generation using Fischer – Tropsch (FT) synthesis<sup>1</sup>. In the present study, we discuss the catalytic route for generation of H<sub>2</sub> in form of syngas by reforming processes such as dry reforming of methane (DR), partial oxidation (PO) and combined reforming or autothermal reforming (ATR) of methane by using Pt, Ru substituted TiO<sub>2</sub> catalysts. Owing to its strong metal support interaction (SMSI), the methane conversions are initiated at low temperatures around 400°C and achieving more than 90% conversions at 700°C by DR process. Unity H<sub>2</sub>:CO ratio is required for the production of oxygenated compounds and liquid hydrocarbons by FT process. With present system of catalysts, we are able to maintain H<sub>2</sub>:CO ratio of 0.95 for a temperature range of 550°C - 900°C.



Besides FT application, we have studied production of high purity H<sub>2</sub> (for PEMFC) for electricity generation. High purity H<sub>2</sub> can be generated by removing CO from the product stream of DR process by water gas shift (WGS) and/or preferential CO oxidation (PROX) process. Regarding this we have synthesized different catalyst system (M/Co<sub>3</sub>O<sub>4</sub> – ZrO<sub>2</sub> (M/CZ)) that provide high oxygen storage capacity, better redox nature and high thermal stability. M/CZ catalyst system is able to remove CO completely below 260°C using WGS technique. As the product stream from reforming process contains varying concentrations of CO<sub>2</sub> and H<sub>2</sub>, the catalytic activity of M/CZ catalyst system was tested with different feed conditions. In addition to WGS, CO removal was studied under PROX conditions (at high concentrations of H<sub>2</sub> in feed). This has given more insight about H – H bond weakening attained on Pt metallic site even at temperatures as low as 100°C, which opened the blindfold of unveiling of our understanding towards a commercial application of hydrogen i.e., catalytic hydrogen combustion (CHC) just at room temperature.

**Keywords:** Reforming; Water gas shift; PROX; CHC

**Reference:**

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**Notes:**

## Modeling the adsorption of fluoride onto activated alumina

*Naga Samrat M.V.V. and K. Kesava Rao*

Water contamination can happen by various anthropogenic and industrial processes. The release of organic and inorganic substances by these processes into water can lead to many diseases upon consumption. Consumption of water containing fluoride ( $F^-$ ) leads to fluorosis and the number of people getting affected with this disease is rapidly increasing in many parts of the world. Adsorption is one of the processes by which defluoridation of water can be achieved. Many adsorbents have been used for defluoridation, including oxides of aluminium, zirconium, lanthanum, iron, magnesium, calcium, etc. These oxides because of their amphoteric nature or because of multiple acidity constants can adsorb/ion-exchange ions. As  $F^-$  is a highly electronegative ion, it can easily adsorb/ion-exchange onto the oxide sites. This process is highly dependent on the pH of the solution to which the adsorbent is exposed. Here we have modelled the batch adsorption/ion-exchange of  $F^-$  onto activated alumina (AA). The approach used is different from that used by many authors, where Langmuir or Freundlich isotherms are used to predict the equilibrium behavior. The latter approach does not show how the different surface species on the oxide surface are affected by the adsorption of  $F^-$ . We have taken the effect of the pH, the surface species, and the ions in solution into account and predicted the adsorption of  $F^-$ .

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**Notes:**

## Lattice Boltzmann for elastic solids

*J.S.N. Murthy and V. Kumaran*

The Lattice Boltzmann Method (LBM) is a numerical method used to solve Navier Stokes equation. Instead of solving the Navier Stokes equations, the discrete Boltzmann equation is solved to simulate the flow of a fluid with collision models such as Bhatnagar-Gross-Krook (BGK). LBM models the fluid consisting of fictive particles, and such particles perform consecutive propagation and collision processes over a discrete lattice mesh. Due to its particulate nature and local dynamics, LBM has several advantages over other conventional CFD methods, especially in dealing with complex boundaries, incorporating of microscopic interactions, and parallelization of the algorithm. LBM is a discrete velocity equation and hence the numerical methods of solution of the system of partial differential equations then give rise to a discrete map, which can be interpreted as the propagation and collision of fictitious particles. However, LBM is not just limited for solving Navier Stokes equation alone. It has been used to solve wave equations, particle suspensions etc.. Here, we apply LB to capture solid mechanics. Since, LB is a method based on discrete particle mechanics, the local interactions should be able to capture the macroscopic physics. The method is applied in such a way that a macroscopic description of the method results in the Navier equations that describe the solid mechanics.

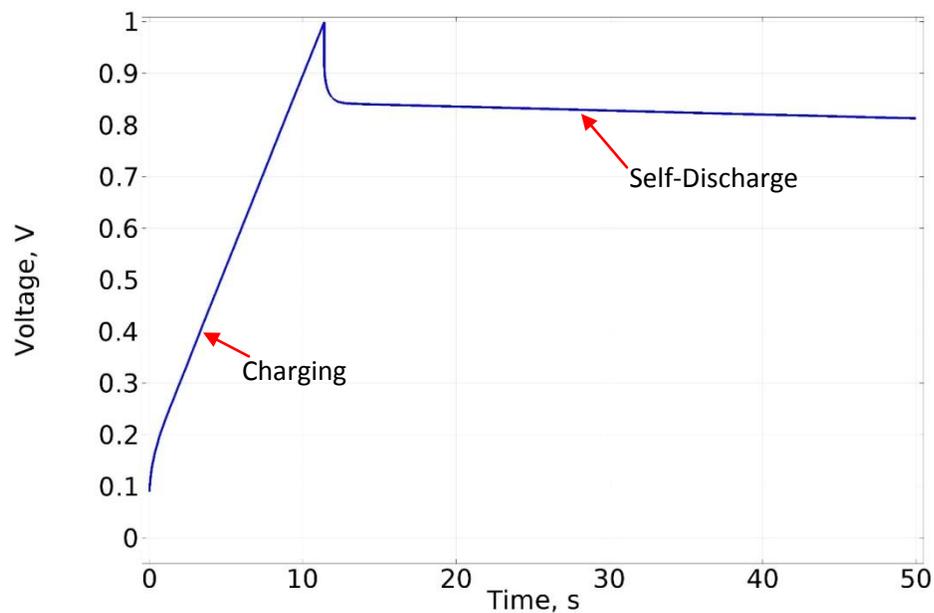
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**Notes:**

## Mathematical modeling of self-discharge in electrochemical capacitors

*Ganesh M. and Sanjeev K. Gupta*

Self-discharge is the loss of stored energy in a device with time during the open circuit condition. It limits the use of electrochemical capacitors as stand-alone energy storage devices in high power applications. Self-discharge is caused by different mechanisms such as charge redistribution, local parasitic reaction or faradaic reactions due to the impurities in electrode or electrolyte. RC circuit models for self-discharge available in the literature are not much helpful in understanding the phenomenon as the models do not involve physical parameters. The transport based models which address the underlying physics for self-discharge are not available in the literature. We have developed a model for self-discharge which can predict the loss of voltage during open circuit conditions. We include floating/leakage current in the model to maintain the device at constant potential or to capture self-discharge under open circuit condition. Figure 1 shows the simulation of the decay of potential after charging from 0V to 1V at  $0.1\text{A}/\text{cm}^2$  for 11.4s and leaving the electrochemical capacitor to open circuit after 11.4s. The present model can explain self-discharge due to charge redistribution, leakage resistance across the interface, floating currents and charging effects using Galvanostatic and Potentiostatic studies which are in agreement with experimental behavior.



**Notes:**

## DSMC Simulation of high mach number turbulent flow in channel

*Aritra Santra and V. Kumaran*

Study of high Mach number compressible gas flow, associated with significant change in density, find its relevance in high-speed aircrafts, jet engines, gas pipelines, combustion reactions and other commercial applications. Typically, flow with Mach number (ratio of flow speed to the speed of sound/thermal velocity) greater than 0.3 falls under the category of compressible flow. The main focus of this work is to characterise turbulence in compressible flow of dilute gas through a channel. We have considered two flow configurations; (i) shear driven flow, (ii) body force driven flow. DSMC (Direct Simulation Monte Carlo) simulation has been implemented to simulate both the flow configurations. DSMC is viewed as a Monte Carlo method for solving time dependent non-linear Boltzmann equation (which describes evolution of dilute gas at the level of single particle distribution function). Reynolds number for transition from laminar to turbulent regime is determined by Linear Stability Analysis. Simulation at higher Reynolds number has been performed by efficient parallelisation of codes using MPI (Message Passing Interface).

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**Notes:**

## Alternative designs to harness natural convection in flow batteries

*Aslam Ansari M.D. and Sanjeev K. Gupta*

Harvesting of renewable energy due to the depletion of conventional energy sources requires researchers to develop efficient energy storage systems. Rechargeable redox flow batteries offer certain advantages over other forms of energy storage techniques in use, such as lifting of water, compression of air, etc. In a redox flow battery, with electrolyte flowing through the space between two electrodes, electrical energy is stored by as chemical energy and vice versa, through reversible reduction-oxidation (redox) electrochemical reactions. Typical applications of these batteries include load-leveling, load shaving, backup power, energy storage, and energy source for electric vehicles. Although some flow battery systems have been scaled up, we are still far from the desired objective--- economical batteries with high energy density, high power density, and long cycle life.

Soluble lead redox flow battery (SLRFB) in its class is the least expensive because of the cost of raw materials and no requirement of expensive proton exchange membrane. However, some challenges such as limited cycle life and low energy efficiency have to be overcome before taking it to the next scale. In our research group, we have established through modeling, electrochemical measurements, and flow visualization that natural convection plays a dominant role. We have harnessed it to develop a new mode of operating a closed SLRFB, in which stirring is provided only during short relaxation stages between charge-discharge cycles. In my work, I am examining various configurations to further promote the role of natural convection and operate these batteries with minimum external stirring. Our simulation results show improvement in charge and energy efficiency in comparison with the previous standard design. Experimental validation of the more efficient design unraveled through COMSOL based simulations is currently underway.

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**Notes:**

**Mechanistic and Kinetic Studies of CO Oxidation over Pristine and Noble Metal Modified Fe<sub>2</sub>O<sub>3</sub> using DRIFTS**

*Disha Jain and Giridhar Madras*

The objective of the present work is to understand the reaction mechanism of CO oxidation on Fe<sub>2</sub>O<sub>3</sub> and noble metal (NM- Pt, Pd) supported and substituted Fe<sub>2</sub>O<sub>3</sub>. Fe<sub>2</sub>O<sub>3</sub> and NM substituted were synthesized by solution combustion technique whereas NM supported Fe<sub>2</sub>O<sub>3</sub> were synthesized by impregnation method. CO oxidation measurements and DRIFTS studies were performed on all the samples. Remarkably, NM supported Fe<sub>2</sub>O<sub>3</sub> were observed to be more catalytically active than the substituted Fe<sub>2</sub>O<sub>3</sub> and the reason for this behaviour was investigated. Pristine Fe<sub>2</sub>O<sub>3</sub>, Pt and Pd supported Fe<sub>2</sub>O<sub>3</sub> showed 100% CO conversion at 280, 180 and 140 °C, respectively. NM supported Fe<sub>2</sub>O<sub>3</sub> exhibited high stability for continuous operation of 24 h, however slight decrease in activity was observed for pristine Fe<sub>2</sub>O<sub>3</sub>, after 10 h of reaction. DRIFTS studies exhibited the presence of solely carbonate species on Fe<sub>2</sub>O<sub>3</sub>. Metal carbonyl bands were observed for NM metal supported Fe<sub>2</sub>O<sub>3</sub> while carbonate bands were seen for Pt supported Fe<sub>2</sub>O<sub>3</sub> but no traces were observed for Pd supported Fe<sub>2</sub>O<sub>3</sub>. Based on the structural characterization and DRIFTS studies, Eley-Riedal mechanism is proposed for Fe<sub>2</sub>O<sub>3</sub> whereas non-competitive and competitive Langmuir-Hinshelwood mechanism is proposed for Pt and Pd supported Fe<sub>2</sub>O<sub>3</sub>, respectively.

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**Notes:**

## Investigating oligomerization pathways of ClyA pore forming toxin (PFT) on artificial bilayer membranes

*Satyaghosh Maurya, Pradeep Sathyanarayan<sup>1</sup>, K. Ganapathy Ayappa, Sandhya S. Visweswariah<sup>2</sup> and Rahul Roy*

*<sup>1</sup>Centre for Biosystems Science and Engineering, IISc Bangalore*

*<sup>2</sup>Dept. of Molecular Reproduction, Development and Genetics, IISc Bangalore*

Pore forming toxins from bacteria form nanoscale lesions on membranes of target cells (~2.5 nm) and results in unregulated efflux of ions and other important biomolecules, finally resulting in cell death. This class of proteins have a unique feature of existing in bi-stable states, i.e., they are produced as water soluble forms and upon exposure to membrane, undergo large scale structural rearrangements, oligomerize and finally result in forming a stable pore. The molecular mechanisms involved in this transition from water soluble state to a membrane integrated pore complex are unknown. The timescales involved in this process are not amenable for investigation using conventional biochemical techniques. Here, we study this process using single molecule imaging techniques that offers us high spatial and temporal resolution to dissect out the pore formation pathway. We also demonstrate how cholesterol is an essential component for effective pore formation and a possible means for selective targeting of PFTs to host cells. Binding and oligomerization of ClyA, a representative PFT from *E. coli* on artificial membrane mimics in the form of supported lipid bilayers was measured in real-time at the single protein level. We find that ClyA binds to these artificial membranes rapidly. From diffusion measurements, we observe a significant population of molecules gradually converting to complexes exhibiting reduced motilities, which could possibly represent pores and other intermediates along the assembly pathway. This effect is accentuated in the bilayers which contain cholesterol. These results are also validated by brightness analysis, wherein two distinct populations are observed as the key step to the assembly dynamics.

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**Notes:**

## Molecular simulation studies on gas hydrates

*Shivanand Kumar and Sudeep N. Punnathanam*

Clathrate hydrates are inclusion compounds in which the host lattice is made up of water molecules connected to each other in a tetrahedral manner via hydrogen bonds. The water lattice contains cavities which are occupied by guest molecules such as methane, ethane, etc. The presence of these guest molecules stabilizes the hydrate by lowering the chemical potential of water in the hydrate phase. The study of clathrate hydrates has been historically important due to their role in blockage of natural gas pipelines. In recent years, their importance has increased, as they play an important role in many scientific and technological areas, such as gas storage and transportation, climate change, and desalination of water. Natural gas hydrates containing methane are also considered as a potential fuel source for the future. The current theoretical understanding of clathrate hydrates is based on the statistical thermodynamic model proposed by van der Waals and Platteeuw known as vdWP theory. The drawbacks of the theory has been corrected using molecular simulations.

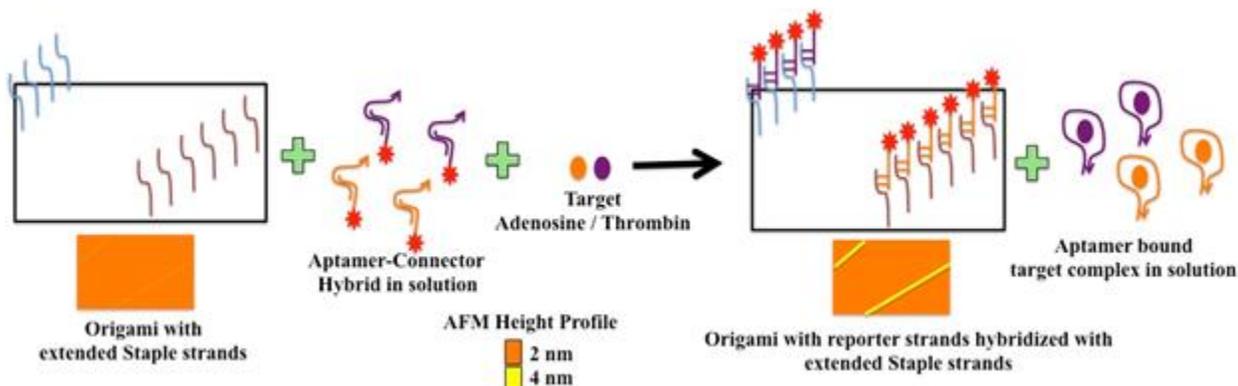
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**Notes:**

## Detection of multiple targets via aptamer binding in solution and reporting with shape specific visual readout on DNA origami surface

*Tulsiram M P, Anusha S and Banani Chakraborty*

With the latest advancement of DNA nanotechnology<sup>1</sup>, specially with the introduction of DNA origami, researchers have widely demonstrated the structural diversity that can be programmed<sup>2</sup> and visualized with various single molecule techniques such as Atomic Force Microscopy (AFM), SEM, TEM, Fluorescence and very recently with single molecule FRET<sup>3</sup>. Recently the functionalizing aspect of DNA origami is being in focus<sup>4</sup>. Here we plan to detect multiple targets such as adenosine, thrombin, lysozyme, kanamycin etc. on a single DNA origami platform. The aptamer-target binding in solution will displace the reporter DNA strand which binds its complementary staple strand as programmed on DNA origami surface (as shown in figure 1). Currently we are testing individual aptamer-target binding in solution using polyacrylamide gel electrophoresis (PAGE), we will follow it up with AFM visualization on origami.



*Figure 1: Schematic representation of multiple aptamer-target binding in solution and reporting on origami surface*

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### Notes:

**Phase transitions under nanoscale confinement : First order or second order?**

*Vadhana V. and K. Ganapathy Ayappa*

Fluids confined in spaces of molecular dimensions exhibit properties different from bulk fluids. Fluid molecules have a tendency to form layers adjacent to a confining solid surface resulting in a transition to a disordered glassy state or an ordered solid-like state. The structuring is quantitatively described by local density variations in the confined geometry, which is a damped oscillatory function of the separation distance between the confining surfaces. In this study, we investigate the state of liquid Octamethylcyclotetrasiloxane (OMCTS), confined between atomically structured mica walls in equilibrium with a bulk reservoir of the same liquid using canonical ensemble simulations. OMCTS confined between mica surfaces has been widely investigated using surface force experiments as well as with molecular simulations assuming a spherical monatomic model. We have carried out simulations using fully atomistic model to investigate possible glassy dynamics. The self-intermediate scattering function is found to decay with increasing relaxation times as the surface separation is decreased and the two-step relaxation in the scattering function, a signature of glassy dynamics, distinctly evolves as the temperature is lowered. The self-diffusivity and relaxation times obtained from the Kohlrausch-Williams-Watts stretched exponential fits to the late  $\alpha$ -relaxation exhibit power law scalings with the packing fraction as predicted by mode coupling theory. Further a freezing point depression of about 30 K was observed for the five layered system. These dynamical signatures indicate that confined OMCTS undergoes a slowdown akin to a fluid approaching a glass transition upon increasing confinement and freezing under confinement would require substantial subcooling below the bulk melting point of OMCTS.

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**Notes:**

## Secondary flow in slow granular flows in a Taylor - Couette viscometer

*Peter Varun D'Souza and Prabhu R. Nott*

Granular media are ubiquitous in both industry and nature, yet there has been no significant headway in understanding their rheological behaviour. In a traditional rheometric device: the Taylor-Couette Viscometer, a puzzling anomaly in the stress profile along the wall was noted.<sup>1</sup> Recent work indicates this is due the presence of a secondary flow.<sup>2</sup> The authors argue these secondary flows are caused by the dilation of the shear band.

We want to see how the magnitude of dilation affects the secondary flows. In this presentation, I will suppress the dilation by confining the system surface. We will show how the secondary flows still persist despite the confining weight, both through DEM simulations and through experiments. We show how the surface of the system changes with and without the confinement. We also show how the shear, if applied via the confining surface, does not lead to secondary flows.

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### Notes:

## Molecular simulation of electric double layer capacitor (EDLC)

*Kaushal Verma and Sudeep N. Punnathanam*

Electrochemical double layer capacitor or supercapacitor is widely used in industries to meet the energy storage demands due to its high power density ( $15\text{kW/kg}^1$ ), long cycle life and wide temperature window. It is an emerging technology and its futuristic applications can be expected in Power buffering, Power saving, Energy recovery, Transport industries and Electronic market. Effective optimization of EDLCs has to consider complicated relationship between electrode and electrolyte properties and its influence on overall power and energy density. However, some experimental observations<sup>1-4</sup> could not clearly understand and interpreted due to limitation of traditional theories<sup>5-7</sup>. Continuum models<sup>8-10</sup> cannot be used to predict capacitance or other properties in devices which employ nanoporous electrodes. An EDLC consists of homogeneous subregions, namely, the positive electrode, the negative electrode and the electrolyte regions, namely, the positive electrode, the negative electrode and the electrolyte region, Gibbs ensemble technique can be used to simulate EDLC with least computational cost<sup>11</sup>. In addition, though the use of grandcanonical ensemble as used in many other studies<sup>12</sup>, simulation of the electrolyte region can be avoided. Electric double layer structure properties of different electrolytes and their comparison in nanoporous electrodes can be made with above tools, Further, there are many important factors influencing electrode capacitance which are difficult to get in experiments like spatiotemporal distribution, change in morphology of electrode due to polarization, which are perhaps easily accessible through computer simulation.

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**Notes:**

## The puzzle of Iridium nanoparticle synthesis

*Phanibhargava V. and Sanjeev K. Gupta*

The reduction of a complex of iridium salt with hydrogen gas leads to the solution sitting with no discernible change of any kind (induction time) for as long as 20 minutes. This phase is followed by a phase of rapid changes, reflected through consumption of iridium precursor and growth of particle size. The two step mechanism of Finke and Watzky, (1997), slow first order continuous nucleation followed by fast autocatalytic particle growth directly from surface reaction of precursor appeared to explain the observations quantitatively, and emerged as a significant breakthrough in the field, after the LaMer model (1950) of particle synthesis. Perala and Kumar (2014), using the rigorous population balance modeling, tested the two-step mechanism and found that it predicts synthesis of highly polydisperse particles, contrary to the observed synthesis of monodisperse particles. A number of alternatives tested by them show that a mechanism that delays the onset of nucleation and quenches it after a time running into tens of minutes is required. They proposed a particles synthesis scheme that had these features. Finke and coworkers (2014) have recently reported, without providing synthesis related measurements, that their first order nucleation rate constant must increase linearly with initial precursor concentration to capture and observed variation in induction time, and have consequently argued for second order nucleation in their two step mechanism, In this work, we have tested the revised two-step mechanism with second order nucleation using the rigorous population balance model. We find that this modification also does not quench nucleation early enough, and the particles synthesized are therefore predicted to be highly polydisperse. Perala and Kumar's reaction scheme which very well captured all the attributes of particle synthesis process cannot be tested rigorously for the new observations due to the non-reporting of the experimental data. Our preliminary efforts, with derived data from the model and the model parameters reported to fit the experimental data, show that Perala and Kumar's scheme also does not capture the observed variation of induction time with precursor concentration. More efforts, both on the experimental and modeling front, are needed to understand the underlying particle synthesis mechanism.

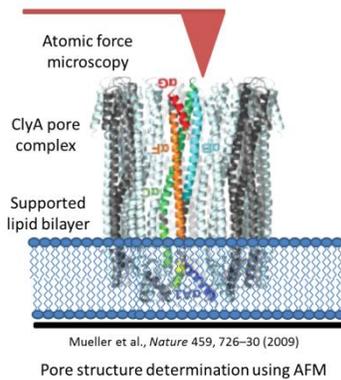
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**Notes:**

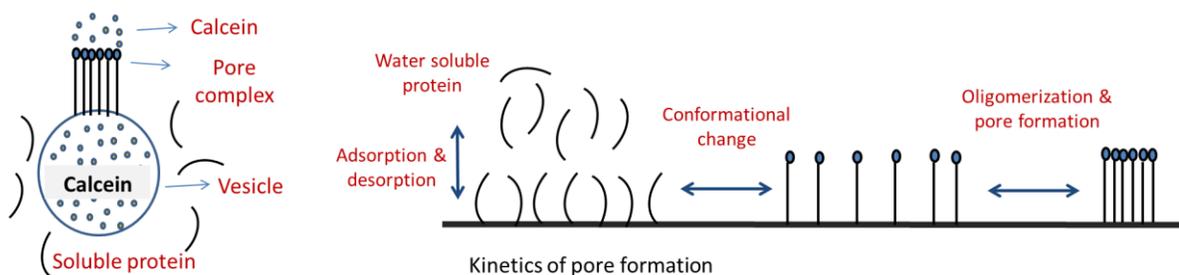
## Interaction studies of pore forming toxins with supported lipid bilayer platforms

*Ayush Agarwal and K. Ganapathy Ayappa*

Observing the structure and dynamics of large protein assemblies on membranes has implications on understanding the general principles behind protein aggregation and engineering drug therapies. Cytolysin-A (ClyA) is a pore forming toxin that is known to cause unregulated pores on various cell membranes. In order to get the structural information of ClyA pore complex, supported lipid bilayers (SLBs) of DMPC were incubated with varying concentrations of ClyA. Pore densities were quantified using atomic force microscopy (AFM).



In the second part of work we have developed a kinetic model for pore formation for calcein leakage experiments, which help us to estimate the time scale for processes such as adsorption, conformational change, oligomerization and pore formation. Upon analyzing the previous studies on PFTs, diffusion of calcein molecule through a pore is not the rate limiting step for pore formation.



**Notes:**

## Motion of a spherical particle near a thin porous slab: An exact solution in bipolar coordinates

*Phanikanth SVSSR and Prabhu R. Nott*

Study of motion of particles near non-porous and porous boundaries has applications in design of micro and nano-fluidic devices and filtration. The motion of a single spherical particle near an impermeable boundary has been studied by several authors [3],[4],[5],[8],[9], but there is no comprehensive study on the motion of a particle adjacent to a permeable boundary. In this study, we consider the motion of a spherical particle near a permeable slab of finite thickness (specifically, in the limit of vanishingly small thicknesses) using analytically simple and computationally less expensive approach [1],[2],[8]. Stokes equations are solved for obtaining the velocity and pressure fields using the bispherical coordinate system. No-slip boundary condition is imposed on the particle surface and a slip condition (proposed by Beavers and Joseph) along with Darcy's flux condition normal to the surface are considered at the porous slab-fluid interface [6],[7]. In addition, we impose the condition of no net flux across the porous slab to obtain the constant non-zero pressure far from slab on the side of the domain not containing the particle. The drag force and torque acting on the spherical particle in the presence of porous slab are computed and compared with those obtained in the presence of a non-porous slab. The effect of various parameters such as distance of the particle center from slab, permeability of slab, slip coefficient and slab thickness is studied.

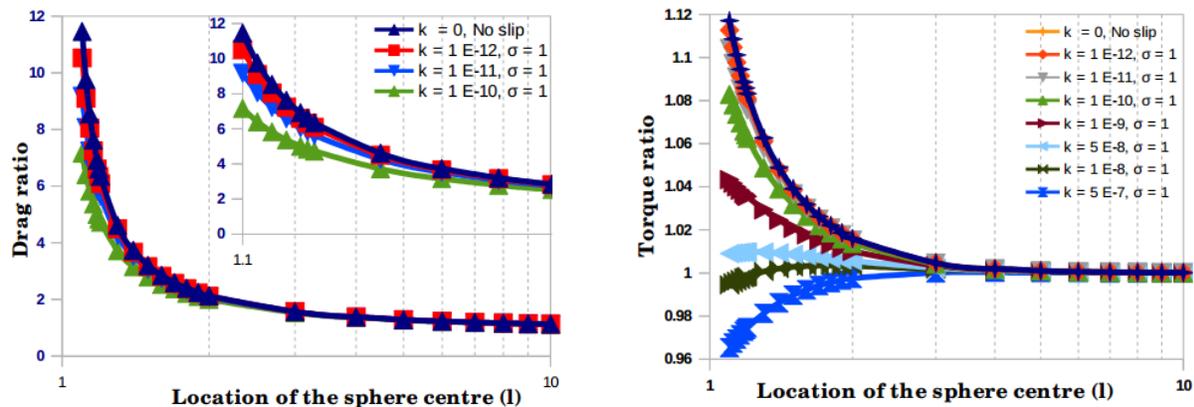


Figure 1. Dimensionless drag and torque acting on a spherical particle near slab a. Translation normal to interface b. Axis of rotation normal to interface

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**Notes:**

## **Esterifying fatty acids with higher alcohols without using a catalyst**

*Ram C. Narayan and Giridhar Madras*

Fatty acid esters of higher alcohols are investigated as potential biolubricants in the past decade. The conventional route involves acid or base catalysts and has several shortcomings such as lower reaction rates due to longer alkyl chains and difficult downstream separations requiring a higher water footprint and associated problems of emulsification. Addressing these issues, an alternative novel pathway is developed for synthesizing these esters. The process involves shifting the phase of the reactant mixture from liquid phase towards a subcritical/supercritical state. At these conditions, the reaction occurs at a much higher rate even without adding external catalysts. In this study, lauric acid and stearic acid (fatty acids) are reacted with n-butanol and isoamyl alcohol at different temperatures (523 K-673 K) and reactant molar ratios (10:1- 40:1). Conversions greater than 85% were obtained within an hour of the reaction. The effect of temperature in increasing the conversion of the fatty acid competes with thermal degradation of esters that occurs at higher temperatures and extended time intervals. The kinetics of esterification was modeled by assuming pseudo first order reaction and activation energies were determined from the Arrhenius plot. The study unravels interesting prospects for biolubricant synthesis using supercritical fluids. Further, ongoing efforts undertaken in this direction and future perspectives are discussed.

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### **Notes:**

## **Effect of morphology of Zinc oxide in ZnO/CdS/Ag ternary nano composite towards photocatalytic inactivation of *E.coli* under visible light**

*Rimzhim Gupta, Jayant M. Modak and Giridhar Madras*

Photocatalytic inactivation of *Escherichia coli* was carried out in the presence of a novel ternary composite of ZnO nanorods-CdS-Ag using UV and visible light. Effect of morphology of ZnO is examined by comparing the photocatalytic activity of nanorods with combustion synthesized nanoparticles and its binary and ternary composites. Ease in charge transfer through uni-direction by nanorods attributes to decrease recombination, found to be the reason of augmented photoactivity of nanorods over combustion synthesized nanoparticles. Visible wavelength absorption is increased by decorating CdS as photosensitizer. Enhanced photocatalysis is achieved by impregnation of 1% Ag on top of the ZnO(NR)-CdS. First order kinetics is observed for all the reactions, which states that rate of inactivation is invariant with initial cell concentration and ZnO(NR)-CdS-Ag is found to give rate constant  $10.99 \pm 0.324$  and  $12.00 \pm 0.628$  h<sup>-1</sup> in UV and visible light respectively. Morphology of synthesized materials was validated by SEM, TEM and crystal structure and lattice parameters were evaluated by X-ray diffraction. Diffused reflectance study was done to ensure the increased absorption by the synthesized composites for superior activity in visible range.

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## Multifunctional $C_3N_4/NiCo_2O_4$ composite for photocatalytic degradation

*Archana C. and Giridhar Madras*

Environmental pollution and energy shortage are serious concerns facing mankind<sup>1</sup>. Designing multifunctional materials may serve as a panacea to such problems. We herein report  $C_3N_4/NiCo_2O_4$  ferromagnetic composite for photocatalytic degradation of Rhodamine B dye. The photocatalysts were characterized by various techniques namely, XRD, SEM, TEM, HRTEM, UV-Vis DRS, photoluminescence and vibrating sample magnetometer (VSM). XRD of composite comprised of both hexagonal phase of  $C_3N_4$  and cubic phase of  $NiCo_2O_4$ . UV-Vis DRS indicated red shift in the absorbance of composite as compared to  $C_3N_4$ . TEM depicts composite as an agglomerated mixture of nanosheets and nanoparticles, having particle size of 50 nm. HRTEM clearly exhibits an interface between  $C_3N_4$  and  $NiCo_2O_4$  confirming the formation of heterojunction between them. Scanning Transmission Electron Microscope (STEM) gives uniform distribution of constituent elements in the composite. The composites had enhanced photocatalytic activity for degradation of Rhodamine B, as compared to  $C_3N_4$  and  $NiCo_2O_4$  under UV irradiation. Superoxide and hydroxyl radicals are major reactive oxygen species involved in photodegradation. Magnetic measurements revealed room temperature ferromagnetism for carbon nitride, nickel cobaltite and the composite<sup>2,3</sup>. Electrochemical measurements were also performed for these materials. Thus, the composites are multifunctional with enhanced photocatalytic performance and room temperature magnetism.

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### Notes:

## Characterizing DNA Aptamer based biosensors using single molecule spectroscopy

*Saurabh Umrao and Rahul Roy*

Everyday the need to detect biologically relevant molecules such as small molecules, proteins, cancer markers etc are increasing and hence the necessity of developing biosensors are on hike for medical diagnostics and biotechnological applications. However, converting the biological information to electronic/optical signal is sometimes challenging because of complex biological environment *in vivo*. This challenge has led the researchers round the globe to develop of biosensors, which employ biomolecules to recognize the cellular target and utilize output elements to translate the biorecognition event into electrical, optical or mass-sensitive signals. Aptamers are single stranded/double stranded DNA molecule that bind their target with high specificity. Aptamers are usually designed through the process named as Systematic Evolution of Ligands by Exponential Enrichment (SELEX)<sup>1</sup>. They have shown added advantage over the antibodies that includes high stability, low cost and simple reagent processing. Moreover, they can be easily fabricated for desired shape and size for biosensor applications. Our current work focuses on an adenosine DNA aptamer that undergoes considerable conformational changes upon cooperative binding of two adenosine (or ATP) with dissociation constant ( $K_d$ ) below  $10\mu\text{M}$ . We have chosen a adenosine aptamer to probe deeper into the mechanistic aspect of the aptamer target binding using “single -molecule Förster resonance energy transfer” (sm-FRET)<sup>2</sup>. The aptamer structure is known to fold and create two pockets for adenosine binding<sup>3</sup>. However detailed conformational and cooperative study of aptamer target binding is yet to be done in most of the cases including adenosine aptamer. Single molecule methods like smFRET not only allow us to measure the conformational changes induced by the ligand binding, but also allows real-time tracking of the structural changes in single molecule level. This gives a strong handle to map the folding/binding pathway, map transient (short-lived) intermediates and dissect the role of each folding step towards the complete binding of the ligand.

We are currently optimising Adenosine aptamer on a generic platform to test any aptamer-target binding in future. We are planning to characterize thrombin DNA aptamer and kanamycin DNA aptamer using same technique and will eventually parallelise the entire

detection procedure on biocompatible surface made of DNA origami<sup>4</sup> to build cost effective multiplexed biosensor on nanobiochip for diseases diagnosis in parallel.

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**Notes:**

## Discrete element modeling to study mechanical behaviour analysis of human hair fibre

*Yogesh Kailas B and Prabhu R. Nott*

Human hair fibre is an amazing natural fibre. It has an unusual behaviour under tensile stress. Stress-strain plot for the fibre shows sequential visco elastic, plastic and strain hardening deformation behaviours. Transition from one behaviour to other happens at well defined strain levels of 2% and 30% respectively. Moreover, hair fibre is structurally similar to semicrystalline polymer, having crystalline rod like segments embedded into amorphous structure. Now the question is how these crystalline and amorphous regions are contributing into the overall behaviour of the fibre. To resolve this problem we are implementing discrete elemental method. Where elastic spring and Newtonian dashpot network is formulated to represent the fibre structure and simulated to get model behaviour similar to the actual hair fibre. Effects of the humidity were also studied on the strength of the fibre.

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### Notes:

## Study of foam stability and bubble size using colloidal particles

*Anukrati Goel and Sanjeev K. Gupta*

Foams are a two phase colloidal dispersion in which gas is the dispersed phase and liquid is the continuous phase. They are thermodynamically unstable as they possess high surface energy. Surfactants are used as conventional foam stabilizer but recently ethyl cellulose particles of around 100 nm diameter have appeared as promising candidates as the foams generated are stable for months. Further, the foam produced by cavitation---recirculation ethyl cellulose solution through a converging-diverging nozzle—consists of bubbles of tens of microns in diameter. At pH 6, the foams produced are unstable as particles carry high negative charge on them, and are unable to adsorb on gas-liquid interface due to large electrostatic repulsion. Lowering of pH increases the stability of foam through lowering of adsorption barrier for ethyl cellulose particles. We have carried out Langmuir trough experiments and disproportionation studies to understand the mechanism of foam stabilization against coarsening.

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**Notes:**

## Dendrimers as nanoscale blocker for the toxic protein pores

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We have used fully atomistic molecular dynamics (MD) simulations to characterize the Cytolysin A (clyA) protein pores modified with fifth generation (G5) PAMAM and sixth generation (G6) PETIM dendrimers. Our results show that the dendrimer, in either of its protonated or nonprotonated form can spontaneously enter the protein lumen to spatially block the protein pores. We observe that the protonated dendrimers strongly couple with the protein wall due to the strong electrostatic interaction between the positively charged dendrimer and negatively charged protein wall. Because of this strong coupling, protonated dendrimers open their branches which eventually block the protein pore more efficiently. On the other hand, charge neutral nonprotonated dendrimers are attached to one side of the pore, thus allowing a free space on the opposite side of the wall. To quantify the effective blockage of the protein pore, we have calculated the ion and water conductance through the protein channel by applying force on the ions/waters. We find that both the ion and water current through the protein pore are remarkably decreased in presence of the dendrimers. However, protonated dendrimer blocks the ionic current more efficiently than the nonprotonated dendrimers because of its specific characteristics. Our investigation shows that the biocompatible PAMAM and PETIM dendrimers can be used as blocking reagent for the pore forming toxins.

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### Notes:

## Millifluidic reactor for room temperature synthesis of gold nanoparticles

*Sushant Kumar and V. Santhanam*

The demand for size controlled Gold colloid with particle sizes in the range of 5-50 nm is expected to be of the order of few tons of gold in weight approximately 1MT in volume for theranostic applications alone. In this context, a mili fluidic reactor has been developed as a first step in scaling up our fed batch protocol for room temperature synthesis of size controlled Gold colloid using tannic acid as reducing agent and stabilizing agent. Our preliminary results indicate that effective mixing plays a critical role in ensuring steady state operation. In this work, we present some salient aspects of our approach.

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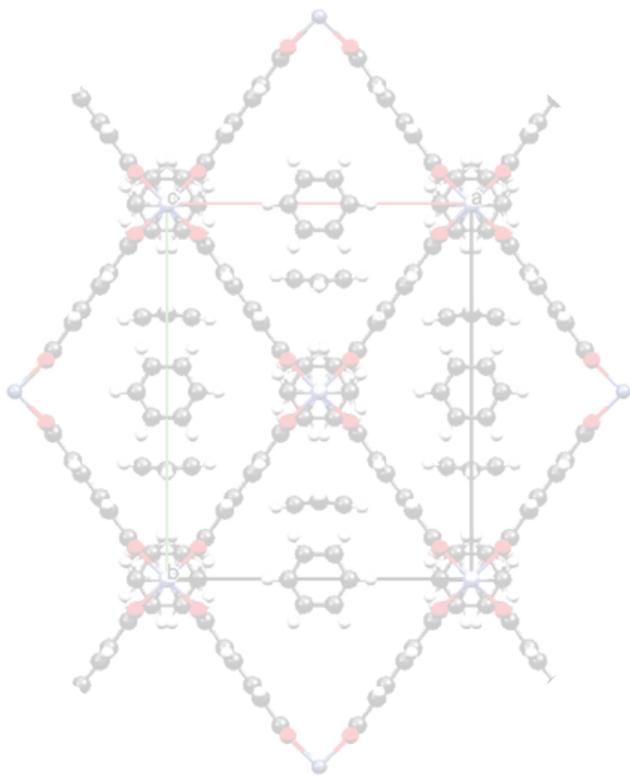
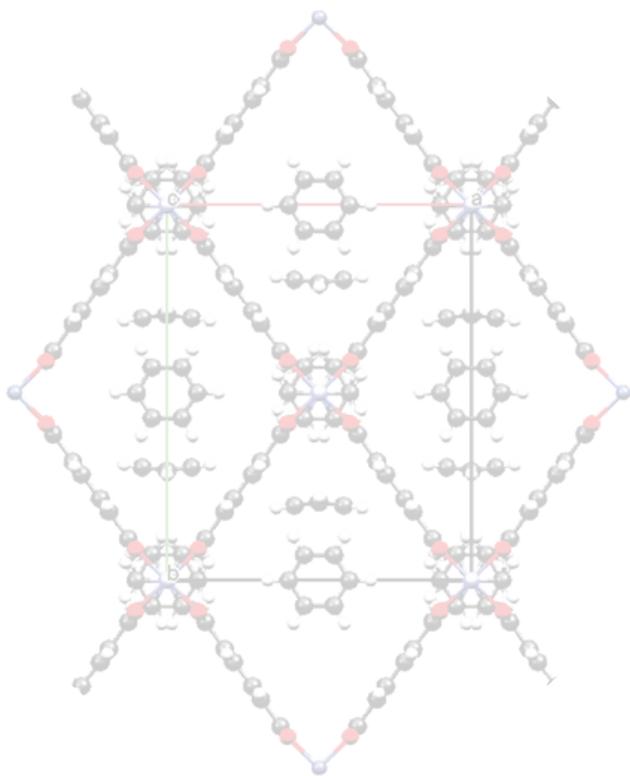
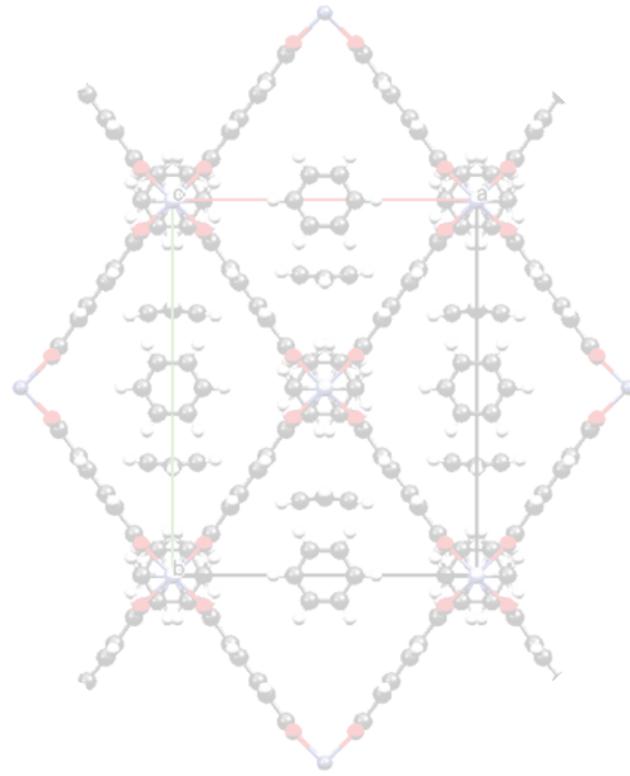
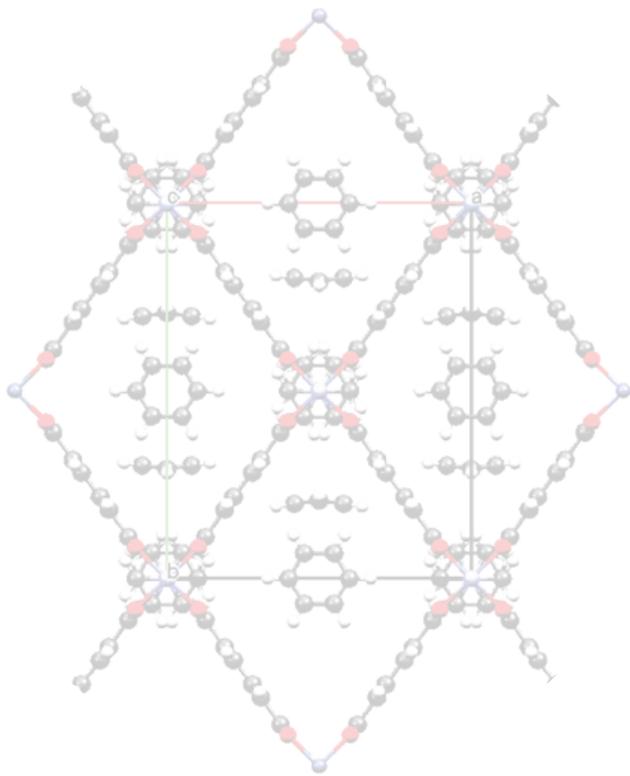
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