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# MOLECULAR SIMULATIONS OF COMPLEX FLUIDS AND INTERFACES



Recent Advances and Challenges

FEBRUARY 21 - 23, 2020  
IIT KANPUR



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# About



## Welcome

Welcome to the international symposium "Molecular Simulations of Complex Fluids and Interfaces", hosted at IIT Kanpur.

The behaviour of interfaces plays an important role in several industrial and natural processes. Molecular simulations can reveal microscopic insights into the structure and properties of solid-liquid interfaces. This meeting aims to provide a forum for exchanging ideas and sharing recent scientific advances from several perspectives. It is hoped that the current state of simulation methodologies will be established, paving the way for the future development of computational tools and research.

## Topics

- Molecular Simulations: New Methodologies and Applications
- Advances in Coarse-Graining and Challenges
- Soft Matter Simulations
- Confined Fluids
- Wetting and Interfacial Phenomena
- Biomolecular Simulations
- Specific Systems and Models

# Timetable

KL: Keynote Lecture, IS: Invited Speaker, ST: Sponsored Talk.

## February 21, Friday

15:00–16:00		<b>Registration</b>	
16:00–16:15		<b>Inauguration Ceremony</b>	
16:15–17:15	KL	<b>Florian Müller-Plathe</b> Technische Universität Darmstadt	Wetting, Drying, Adhesion
17:15–17:40	IS	<b>Neelanjana Sengupta</b> IISER Kolkata	Modulating Self-Assembled Amyloidogenic States via Solvent and Temperature: Insights from Computer Simulations
17:40–18:05	IS	<b>Harshwardhan Katkar</b> IIT Kanpur	Multiscale Modeling of Actin Filaments
18:05–18:30	IS	<b>Manjesh K. Singh</b> IIT Kanpur	Rheology of Nonequilibrium Polymer Melts
19:00–21:30		<b>Reception Dinner</b>	

## February 22, Saturday

9:30–10:30	KL	<b>Edward Maginn</b> University of Notre Dame	Computational Design of New Materials for Separations and Energy Storage
10:30–11:00	<b>Tea Break</b>		
11:00–11:25	IS	<b>Beena Rai</b> Tata Research Development and Design Center	Skin Lipids and their Interfaces: A Computational Approach towards Mimicking Skin Barrier Function
11:25–11:50	IS	<b>Sudip Roy</b> National Chemical Lab, India	Bridging Scales for Simulation of Lipids
11:50–12:15	IS	<b>Swati Bhattacharya</b> IIT Bombay	Molecular Dynamics Investigations of anti HIV-1 protein SAMHD1
12:15–12:40	IS	<b>R. Sankararamakrishnan</b> IIT Kanpur	TBA
12:40–14:00	<b>Lunch Break</b>		
14:00–15:00	KL	<b>Balasubramanian Sundaram</b> JNCASR	Modelling Supramolecular Polymers
15:00–15:25	IS	<b>Divya Nayar</b> IIT Kharagpur	Microscopic View of the Crowding Effects on Hydrophobic Collapse
15:25–15:50	IS	<b>Nisanth N. Nair</b> IIT Kanpur	Exploration of High Dimensional Free Energy Landscapes of Chemical Reactions
15:50–16:20	<b>Tea Break</b>		
16:20–16:45	IS	<b>Rajat Srivastava</b> Politecnico di Torino	Thermo-Physical Properties of Graphene Reinforced Thermoplastics: A Coarse-Grained Modelling Approach
16:45–17:10	IS	<b>Tamal Banerjee</b> IIT Guwahati	Reactive Force Field Simulations on the Degradation of Quinoline
17:10–17:30	ST	<b>Ashwini Kumar</b> NEC Corp.	Vector Computing- Simulation and A.I.
17:30–18:55	<b>Poster Presentation Session</b>		
18:55–19:00	<b>Announcement of Springer Best Poster Awards</b>		

## February 23, Sunday

9:30 –10:30	KL	<b>David A. Kofke</b> SUNY, Buffalo	'Mapped Averaging' Method for deriving Ensemble Averages: Application to Crystals
10:30–11:00	<b>Tea Break</b>		
11:00–11:25	IS	<b>Shantanu Maheshwari</b> Shell Technology	Nucleation and Growth of a Nanobubble on Rough Surfaces
11:25–11:50	IS	<b>Kaustubh Rane</b> IIT Gandhinagar	The Role of Solid-Liquid Interfacial Fluctuations in the Spontaneous Motion of Droplets
11:50–12:15	IS	<b>Sandip Khan</b> IIT Patna	The Wetting Behavior of Imidazolium Based Ionic Liquids using Molecular Dynamics Simulation
12:15–12:40	IS	<b>Jhumpa Adhikari</b> IIT Bombay	Phase Equilibria of Binary Mixtures of Triangle-Well Fluids : Bulk vs Confined Systems
12:40–14:00	<b>Lunch Break</b>		
14:00–14:25	IS	<b>Sudeep Punnathanam</b> IISC Bangalore	Computing Solid-Liquid Interfacial Free Energy via Thermodynamic Integration
14:25–14:50	IS	<b>Subir K. Das</b> JNCASR	Kinetics of Clustering in an Assembly of Vicsek-Like Active Particles
14:50–15:15	IS	<b>Tarak Patra</b> IIT Madras	Correlation between Glass Formation and Ion Conductivity in Polymeric Ionic Liquids
15:15–15:40	IS	<b>Prateek Kumar Jha</b> IIT Roorkee	Multiscale Modeling Approaches in Excipient Design for Oral Drug Delivery
15:40–16:10	<b>Tea Break</b>		
16:10–16:35	IS	<b>Sk. Musharaf Ali</b> BARC, Mumbai	Microscopic Assessment of Liquid-Liquid Extraction System in Bulk and at the Interface
16:35–17:00	IS	<b>Vishwanath Dalvi</b> ICT, Mumbai	Study of Water Extraction by Phosphate Ligands by Experiments and Molecular Simulations
17:00–17:25	IS	<b>Rajat Desikan</b> Invictus Oncology Pvt. Ltd.	Accurate Computational Calorimetry of Lipid Membranes by void-induced Melting
17:25–17:35	<b>Springer Poster Awardee Talk-1</b>		

17:35–17:45	<b>Springer Poster Awardee Talk-2</b>
17:45–18:00	<b>Vote of Thanks</b>
19:00–21:30	<b>Symposium Dinner</b>

# List of Abstracts – Talks

**February 21, Friday**

## **Wetting, Drying, Adhesion**

**F. Müller-Plathe**

**KL**

Technische Universität Darmstadt

We will review recent advances on the simulation of small-molecule fluids as well as polymers at solid interfaces. We will cover wetting of surfaces by liquids as well as the evaporation of liquid droplets from them. We will also look at the structure formation of polymers near solid surfaces and the resulting interphase properties, such as encountered in coatings and nanocomposites.

# **Modulating self-assembled amyloidogenic states via solvent and temperature: Insights from Computer Simulations**

**N. Sengupta**

IS

Department of Biological Sciences, Indian Institute of Science Education and Research  
Kolkata, India

Self-assembled amyloid conformations are more resistant to ‘denaturation’ than the folded states of globular proteins. This corresponds, in large part, to the nature of their conformational energy landscape. Folding is typically associated with a rough, yet ‘funnel-shaped’ energy landscape corresponding to an identifiable conformational minimum. In contrast, the landscape corresponding to amyloid formation features several equivalent minima separated from highly stable ‘amyloid’ conformations by large kinetic barriers. A recurring challenge in protein biophysics has been to identify perturbative ways to disrupt stable amyloids; consequences range from proteopathic amelioration to preservation of bio-specimens. Such goals, however, necessitate molecular-level details of the response of the amyloidogenic assemblies to perturbative conditions. Herein, I will highlight first our efforts toward understanding the effects of a cosolvent in interfering with early amyloid assembly. I will then discuss our recent work on thermal conditions affecting the stability of a putative pre-formed amyloid; the overall structural response is decoupled from the thermodynamic response of the hydrophobic core, contradicting the expectations of a folded state. Further work reveals that these effects are modulated by the hydration layer in proximity to the amyloid states; this layer contains important signatures of the overall structural and thermodynamic response.

## February 22, Saturday

### Computational Design of New Materials for Separations and Energy Storage

E. J. Maginn

KL

Department of Chemical and Biomolecular Engineering, University of Notre Dame

Chemical separation technologies such as distillation account for tremendous amount of the world's energy consumption. As a consequence, the National Research Council has called for the development of alternatives to distillation to meet the Energy Intensity of Chemical Processing Grand Challenge. In the first part of this talk, I will focus on ionic liquid solvents designed to preferentially separate CO<sub>2</sub> from air, methane and hydrogen. Permeabilities / separation factors are computed for ionic liquids confined in membranes and in nanoporous media. The solubility of chemically reacting ionic liquids is computed directly using a combination of quantum and classical modeling approaches. A new reactive Monte Carlo (RxMC) method is described that enables the direct calculation of the reactive absorption isotherm as a function of pressure. Energy storage technologies such as rechargeable batteries are key enablers of renewable energy sources such as wind and solar. The development of "beyond lithium ion" batteries relies upon the development of new electrolytes. In the second part of the talk, I will describe our work simulating "water-in-salt" electrolytes and deep eutectic solvent electrolytes, where we compute the structure and dynamics of these systems and compare with results from experimental collaborators.

## **Skin Lipids Their Interfaces: A Computational Approach Towards Mimicking Skin Barrier Function**

**B. Rai**

IS

Tata Research Development and Design Center, India

Human skin is a vital organ acting as an interface between us and our surroundings. It is one of the largest organ of our body comprising of three layers – Epidermis, Dermis and Hypodermis. While epidermis is responsible for overall appearance and texture of skin, its outermost layer called stratum corneum (SC) controls its barrier function. Dermis, primarily made up of collagen and elastin, provides structural support and elasticity. The deepest layer – hypodermis, is composed of adipose tissues and provides the heat resistance. SC is composed of 15–20 layers of flattened cells called corneocytes (Bricks) which are embedded in a lipid matrix (Mortar) composed of ceramides, cholesterol, and fatty acids. The “bricks and mortar” structure of SC makes it selectively permeable thus protecting underlying tissue from infection, dehydration, chemicals and mechanical stress. While corneocytes of SC remain almost impermeable, 95

## **Molecular Dynamics Investigations of Anti HIV-1 Protein SAMHD1**

**S. Bhattacharya**

IS

Indian Institute of Technology Bombay, India

HIV-1 is restricted in macrophages and certain quiescent myeloid cells due to a “Scorched Earth” dNTP starvation strategy attributed to the Sterile Alpha Motif and HD domain protein – SAMHD1. Active SAMHD1 tetramers are assembled by GTP-Mg<sup>2+</sup>-dNTP cross bridges and cleave the triphosphate groups of dNTPs at a Km of 10 uM, which is consistent with dNTP concentrations in cycling cells, but far higher than the equivalent concentration in quiescent cells. HIV-2 and SIV have evolved defences against SAMHD1, underscoring its role in restriction. The regulation of SAMHD1 by phosphorylation (at T592) and Glutathione driven redox reactions has been experimentally studied and yet not properly understood. We have used correlation network analysis along with molecular dynamics techniques to study the flow of allosteric information across the active complex. I will discuss how our MD analysis has yielded insights that complement and expand X-Ray and biochemistry based models of SAMHD1 activity.

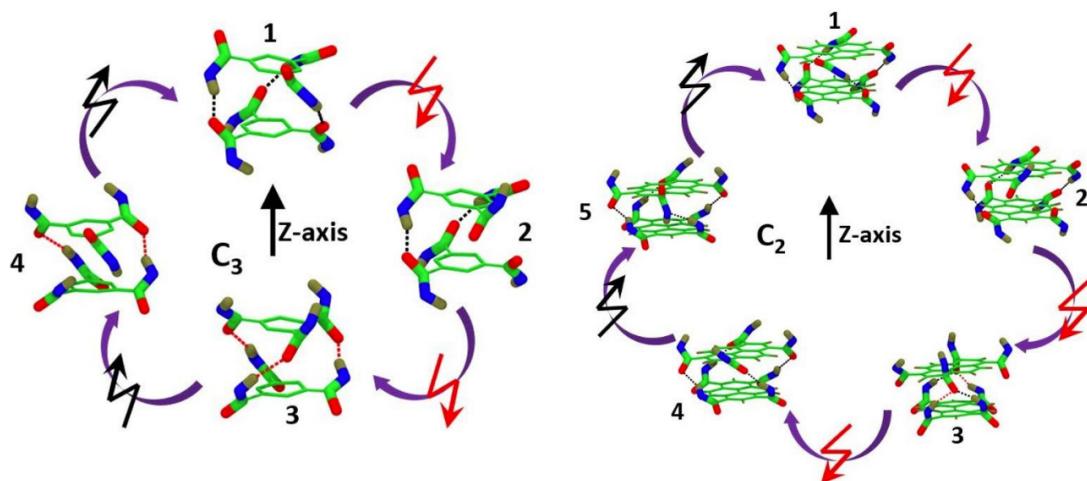
# Modelling Supramolecular Polymers

B. Sundaram

KL

Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru

Unlike conventional polymers, supramolecular polymers are formed out of non-covalent interactions between monomers in solution. The relatively weaker interaction strengths makes the association between the monomers to be reversible. Molecular simulations are apt to study this self-assembly process as they possess the right tools to take into account finite temperature and bulk solvent conditions explicitly. The talk will review the vast experimental literature on this topic and will introduce the computational techniques. The application of such methods have led to the following new findings: ground state dipole configuration in the classic BTA system, dipole driven cooperative mechanism of polymerisation, reversal of chiral handedness concomitant with polarization reversal in ferroelectric thin films of supramolecular polymers, and the demonstration of isodesmicity in self-assembly, using free energy methods.



# Microscopic View of the Crowding Effects on Hydrophobic Collapse

D. Nayar

IS

Centre for Computational and Data Sciences, IIT Kharagpur, India

A living cell is a crowded milieu comprising of large-sized macromolecules, small co-solutes and ions with less free water [1,2]. Crucial biological processes involving hydrophobic collapse such as protein folding and other self-assemblies occur in this environment. However, a molecular-level understanding of these effects remains elusive. It has been widely accepted that these effects are induced due to size (steric) effects of crowders and the solvent excluded volume effects that are entirely entropic in nature [1]. This excludes the role of any direct solute-crowder or crowder-crowder attractive interactions, which however has been shown to play a crucial role recently [3]. Therefore, molecular mechanisms associated with these effects need to be further explored. We investigate the crowding effects of small (tri)peptides on collapse equilibria of a generic hydrophobic polymer. Advanced molecular dynamics simulations and statistical mechanics solvation theories are used to examine solvation thermodynamics of polymer collapse. The unresolved role of crowder intermolecular interactions is examined. Our results show that weak polymer-crowder attractions lead to strong polymer collapse only at high crowder volume fractions, involving entropic depletion of crowders from polymer surface, in accordance with the widely known depletion mechanism. Interestingly, on making the polymer-crowder attractions stronger, polymer collapses at low volume fractions and that too via preferential adsorption of the crowders on the polymer surface. Strongly interacting crowders weaken the polymer collapse at high crowder volume fractions. A transition from enthalpy-dominated to entropy-dominated polymer collapse is observed with increasing crowder concentrations. Our results provide new insights into the existing theories of crowding effects on macromolecular collapse and the talk will discuss its implications on macromolecular collapse/aggregation processes.

## References

- [1] Zhou, H.-X.; Rivas, G. ; Minton, A.P. *Annu. Rev. Biophys.* 2008, 37, 375-397.
- [2] Wang, K.-H.; Chang, C.-W. *Phys. Chem. Chem. Phys.* 2015, 17, 23140–23146
- [3] Sukenik, S.; Politi, R.; Ziserman, L.; Danino, D.; Friedler, A.; Harries, D. *PloS ONE*, 2011, 6, e15608.

## Reactive Force Field Simulations on the Degradation of Quinoline

T. Banerjee

IS

Department of Chemical Engineering, IIT Guwhati, India

In the current study, quinoline is considered as a model Poly Aromatic Hydrocarbon where Reactive Force Field (ReaxFF) simulations is adopted to study its degradation and pyrolytic behaviour. To confirm the intermediate and final products, a range of ReaxFF MD simulations at different temperatures with NVT ensembles for a total duration of 700 ps were implemented. Five different temperatures ranging from 2500 K–4500 K are chosen so as to allow the chemical reactions to be observed at a computationally affordable time scale. We observed a qualitative experimental agreement with respect to initiation step of the quinoline hydrogenation and formation of major intermediate products such as Tetrahydroquinoline (THQ), Propylaniline (PA) and decahydroquinoline (DHQ). Most of the intermediate reactions are found to be intramolecular while intermolecular reactions dominate at higher temperatures. The main products include ammonia, ethylene, methane, ethane and acetylene. Finally, a kinetic analysis was made to obtain the rate constants and activation energies for quinoline hydrogenation.

## February 23, Sunday

### The Role of Solid-Liquid Interfacial Fluctuations in the Spontaneous Motion of Droplets

**U. Saxena, S. Chouksey, K. Rane**

IS

Indian Institute of Technology, Gandhinagar, India

The density fluctuations at the solid-liquid interfaces have received great attention in recent decades in the context of protein folding. In this presentation, I will discuss them in the context of droplet motion on heterogeneous surfaces. I will first discuss our efforts to understand how the above fluctuations affect the variation of solid-liquid interfacial free energy with the nature of crystalline surface. We used the grand canonical Monte Carlo (GCMC) simulations and the cumulant expansions of the interfacial free energy to relate the above fluctuations to the interfacial entropy [1]. We observed that interfacial entropy is important for the motion of droplets when the temperature varies spatially, or temporally. I will also discuss a model system where the fluctuations are expected to strongly affect the motion of droplet [2]. Here, we used the molecular dynamics simulations to study the motion of droplet, and GCMC simulations to compute the interfacial free energies. I will end the talk by discussing our efforts to rationally design the solid surfaces having the desired solid-liquid interfacial fluctuations by using the principle of Maximum Entropy.

#### References

- [1] Chouksey, S., Rane, K. Transverse correlations near solid-liquid interface: Influence of the crystal structure of solid. *Chemical Physics* 517, 188–197 (2019).
- [2] Saxena, U., Chouksey, S., Rane, K. Spontaneous translation of nanodroplet over a heterogeneous surface due to thermal cycles: role of solid–liquid interfacial fluctuations. *Molecular Physics* 1–14 (2019). doi:10.1080/00268976.2019.1657191

# Computing solid-liquid interfacial free-energy via thermodynamic integration

R. K. Reddy, S. N. Punnathanam

IS

Department of Chemical Engineering, Indian Institute of Science, Bengaluru 560012, India

In this talk, we present a method to compute solid-solvent interfacial free-energies for sparingly soluble solutes via thermodynamic integration. The proposed method combines the phantom-wall method of Leroy and Muller-Plathe [1] and the Frenkel-Ladd method [2] for solid-state free energy calculation. Our proposed method included the contribution of entropy of both solid and liquid phases in the computation of the interfacial tension. We apply this method to predict the influence of solvent on polymorph selectivity during crystal nucleation of molecular solids and vapor-liquid contact angles on a solid substrate. The proposed method for computing interfacial tension can be easily implemented using the open-source molecular dynamics package LAMMPS. This can facilitate widespread adoption of this method by a large number of research groups.

## References

- [1] J. Chem. Phys. 133, 044110 (2010)
- [2] J. Chem. Phys. 81, 3188 (1984)

# **Microscopic Assessment of Liquid-Liquid Extraction System in Bulk and at the Interface**

**A. Das<sup>1,3</sup>, P. Sahu<sup>2,3</sup>, Sk. M. Ali<sup>2,3</sup>**

IS

<sup>1</sup> Nuclear Recycle Board, Bhabha Atomic Research Centre, Trombay, Mumbai, India

<sup>2</sup> Chemical Engineering Division, Bhabha Atomic Research Centre, Trombay, Mumbai, India

<sup>3</sup> Homi Bhabha National Institute, Trombay, Mumbai, India

The recent trend toward renewal of interest in nuclear power as a futuristic energy alternative demands a close cycle spent fuel reprocessing methods with a long term vision for safe management of spent fuel. Nuclear fuel cycle is important not only to reduce the high-active solid waste but also to produce the fresh fuel for 2nd generation nuclear reactor. The extent of reprocessing depends on the efficiency of the liquid-liquid extraction processes in which the radionuclides are separated from acidic aqueous solution. The most extensively used solvent in spent fuel reprocessing is tri-n-butyl phosphate (TBP) with n-dodecane as the diluent in the PUREX process. In spite of great success, there is a demand and continuing search for an alternative of TBP, specifically for spent fuels from fast breeder reactor. Among many, tri-isoamyl phosphate (TIAP) has been considered as competitor which has similar chemical and radiological stability like TBP in presence of nitric acid. In this context, thermo-physical and dynamical properties of ligand-solvent systems are required to predict the extraction efficiency for a representative system which can be obtained either by performing experiments or by molecular dynamics (MD) simulations. In that perspective, MD simulations assist to arrive at a reasonable conclusion in minimum no of trials of experiments and thus reduce the cost as well as time. Furthermore, there is a continuing endeavour at the molecular level understanding of liquid-liquid bi-phasic extraction of metal ions due to its wide level of application from pharmaceuticals to nuclear industry. Microscopic understanding of the interface between two immiscible or partially miscible liquids of any biphasic system not only has a great interest in view of mass transfer processes but also has considerable technological values in the field of chemistry, physics and biology. Due to inherent difficulty, the understanding of molecular details at liquid-liquid interface using only experimental technique is inadequate to establish the interfacial behaviour. This is mostly due to the fluidity of the interface and its concealed environment, which restricts the experimental facts. The contribution of intrinsic thickness and broadening induced by capillary waves are responsible for total thickness but the determination of these two values are perhaps not encountered for three component system. MD simulations provide a microscopic analysis of the interfacial properties of water-organic interface. The present talk will focus on evaluation of structural, thermo-physical and dynamical properties of the liquid-liquid extraction system in bulk and at the interface using molecular dynamics simulations.

## **References**

- [1] Sk. Musharaf Ali, A Boda, AKS Deb, P Sahu, KT Shenoy, Computational Chemistry Assisted Design and Screening of Ligand-Solvent Systems for Metal Ion Separation, *Frontiers in Computational Chemistry*: , 2017, Volume: 3 3, 75, Bentham Science.
- [2] P Sahu, Sk. Musharaf Ali, KT Shenoy, *Physical Chemistry Chemical Physics*, 2016, 18, 23769-23784.
- [3] A. Das, P. Sahu, Sk. Musharaf Ali, *J. Chem. Eng. Data* 2017, 62, 22802295.
- [4] Arya Das and Sk. Musharaf Ali, *J. Chem. Phys.* 2018, 148, 074502.
- [5] A. Das, Sk. Musharaf Ali, *Journal of Molecular Liquids*, 2019, 277, 217–232.
- [6] A. Das, Sk. Musharaf Ali, *J. Phys. Chem. B*, 2019, 123, 21, 4571-4586.

# List of Posters

## Tuesday Session

# Molecular Dynamics Simulations on Interfacial Structure in Presence of Third Component

A. Das<sup>1,3</sup>, Sk. M. Ali<sup>2,3</sup>

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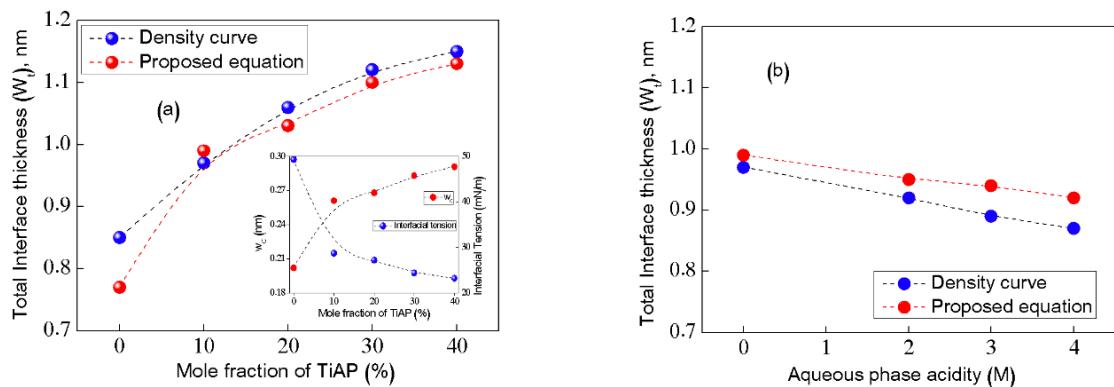
Microscopic understanding of the interface between two immiscible or partially miscible liquids for a biphasic system not only has an immense interest in view of mass transfer processes but also has significant technological importance in the field of science and engineering. Due to its inherent difficulty, the understanding of molecular details at liquid–liquid interface using only experimental technique is not enough to ascertain the interfacial behaviour mostly due to the fluidity of the interface and buried surroundings. The contribution of intrinsic thickness and broadening induced by capillary waves ( $w_c$ ) are responsible for total thickness but their determination are perchance not encountered for three components system. In this context, we have performed molecular dynamics (MD) simulations of a technologically important water–dodecane system containing tri-isoamyl phosphate (TiAP) used for reprocessing of radionuclide. MD simulations provide a microscopic view of the interfacial properties of water–dodecane/TiAP interface. Further, an empirical relation between interfacial tension and interface thickness has been established for water–dodecane/TiAP system [1] (see inset of Fig. 1) which is also related by capillary wave theory (CWT) as:

$$w_c^2 = \frac{k_B T}{2\pi\gamma} \ln \left( \frac{L_{II}}{L_b} \right)$$

Here,  $k_B$  is Boltzmann constant and  $T$  is temperature,  $L_{II}$  is the box dimension along  $x$  or  $y$  direction.  $L_b$  represents bulk correlation length commonly expressed in terms of molecular length which is evaluated from the volume determined by COSMOtherm program at the BP/TZVP level of theory as implemented in Turbomole package. The calculated  $w_c$  for water–dodecane system [1] (0.202 nm) is in good agreement with reported (0.338nm) results [2]. For a three components system, it is reasonable to introduce the weighted average of dodecane and TiAP for determination of Lb to account the effect of TiAP. Furthermore, the total interface thickness ( $w_t$ ) cannot be solely represented by  $w_c$ . The wt can be empirically fitted as [1]:

$$w_t^2 = \frac{(\sigma_{water} + \sigma_{TiAP} + \sigma_{dodecane})}{1.4\sigma_{water}} \frac{k_B T}{\gamma} \ln \left( \frac{L_{II}}{L_b} \right)$$

The total interface thickness obtained from density curve and Eq. (2) are in good agreement as shown in Fig. 1 as a function of mole fraction of TiAP and acid concentration. Eq. (2) might be useful for determining  $w_t$  for a wide range of bi-phasic system.



$W_t$  from density curve and Eq. (2) as a function of (a) mole fraction and (b) aqueous phase acidity.  $W_c$  and vs. mole fraction of TiAP [inset of Fig. (a)]

## References

- [1] A. Das, Sk. M. Ali, J. Mol. Liq., 2019, 277, 217–232.
- [2] D. M. Mitrinovic, A. M. Tikhonov, M. Li, Z. Huang and M. L. Schlossman, Phys. Rev. Lett. 2000, 85, 582.

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