

## **Ionic Liquid Mediated H-bond interactions to modulate the structure and properties of self-aggregated system: A combined experimental and computational study**

### **Abstract:**

Effect of hydrogen bonding interaction is ubiquitous in the field of self-aggregated systems. The present study represents the effect of Ionic Liquid (IL) mediated extensive H-bonding interaction on microemulsion (ME) stability, drug reformulation and hydrogel synthesis. Ionic Liquids (IL) are a class of task specific low melting salts of organic cations and anions. We synthesized a series of ILs with guanidinium, cholinium and imidazolium cations and characterized those. However, only guanidinium ILs imparted higher stability of water-in-oil microemulsions (ME) through the formation of interfacial H-bonding network at the water/oil interface. Further, the presence of IL triggered the percolation behavior in the ME via dynamic droplet collisions. Next, we reformulated insoluble/sparingly soluble Active Pharmaceutical Ingredients (APIs) by conjugating those with guanidinium and cholinium cations. Thus, the API-ILs having high solubility and sufficient permeability could be delivered in liquid formulations with better compliance particularly to the pediatric and geriatric class of patients. *In-vivo* testing results on rat model also suggested probable rapid onset of API-ILs compared to the parent APIs. The last part of the work was to introduce guanidinium cations as cross-linker into the structural framework of alginate polymer which produced soft and adhesive hydrogels. The cross-linked hydrogel, in conjunction with *in-situ* synthesized silver nanoparticles, evidenced excellent antibacterial coating properties against gram-positive and gram-negative bacteria. Additionally, the free-standing film from cross-linked hydrogel is being tested as a topical therapeutic patch for wound healing. Thorough experimental investigations and computational studies were performed to have detailed understanding on aforementioned systems.