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Wetting Behavior and Interfacial Dynamics of Aqueous Deep Eutectic Solvents on Diverse Substrates through Molecular Dynamics Simulations: Implications for Enhanced Oil Recovery and Sustainable Applications

Alok Kumar[1], Swasti Medha[1], Devargya Chakraborty[1*], Debashis Kundu[2], Sandip Khan[1]

[1]Department of Chemical & Biochemical Engineering, Indian Institute of Technology Patna, Patna 801106, India.

[2]Department of Chemical Engineering, ICT Jalna, India

* Corresponding Author's Email ID: devargya_2021cb02@iitp.ac.in

ABSTRACT

The wetting behavior and interfacial properties of aqueous Deep Eutectic Solvents (DES) on a variety of substrates, including graphite, silica, and calcite surfaces, were examined in this study using molecular dynamics simulations. In particular, we investigated two different DES compositions distributed in aqueous solutions: Choline Chloride-Urea (CCU) and Choline Chloride-Ethylene Glycol (CCEG) at a 1:2 ratio. The goal of our work was to comprehend the intricate molecular interactions that underlie wetting occurrences on these various substrates. A thorough examination of the molecular interactions between various molecules and the substrates was carried out in order to gain a profound understanding of the equilibration process of DES droplets on these surfaces. In-depth contact angle measurements on graphite and silica surfaces were part of later investigations. Our results revealed intriguingly low contact angles on calcite surfaces, around 10 degrees, which prompted a thorough investigation using thin film analysis to clarify the interesting behavior displayed by DES on calcite surfaces. Initiating our investigation, we examined density distribution patterns of distinct molecules within the aqueous DES mixtures. This was followed by an extensive hydrogen bond analysis, crucial for unraveling the fundamental mechanisms governing wetting behavior. Significantly, our results emphasized the prevalence of water-water hydrogen bonding within aqueous DES mixtures, highlighting the pivotal role of hydrogen bonds in shaping observed wetting phenomena. The results of this study have broad implications for the possible use of DES molecules in a variety of fields. Our findings provide new opportunities for utilizing DES in enhanced oil recovery techniques, which are particularly pertinent in areas with a high concentration of calcite-rich rocks that are known to contain significant oil reserves, like some parts of India. Additionally, the sustainability and environmental friendliness of DES make them attractive candidates for enhancing the potential and adaptability of these solvents.

Keywords: Wetting behavior, Deep Eutectic solvent, Molecular dynamics simulation, Enhanced oil-recovery, Hydrogen bonding

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