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Effect of counterion on the self-assembly of N-hydroxy alkyl ammonium surfactants

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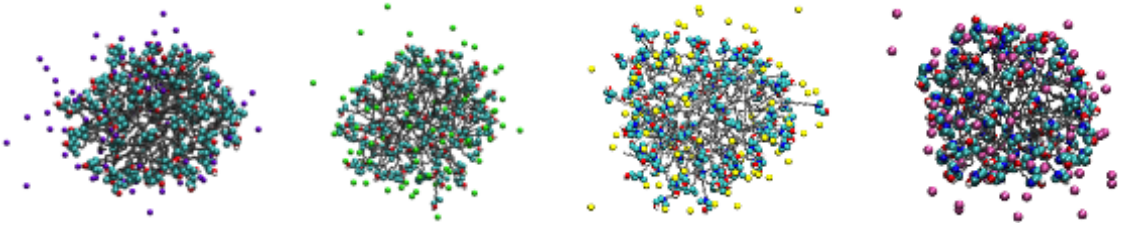
Abstract: Surfactants are amphiphilic molecules and find application in almost every chemical industry, like as detergents, paints, cosmetics, pharmaceuticals and used for environmental protection [1]. This lack of applications is due their physicochemical properties that gives them the ability to promote aggregation and interaction with different interfaces [2,3]. Our goal is understanding how the nature of counterion change the properties of aggregation. In this study, we investigate how this important property of aggregation varies for cationic surfactants molecules of N,N-dimethyl-N-alkyl-N-(hydroxyethyl) ammonium salt (HEA^+) with different counterions as fluoride, chloride, bromide and iodide using molecular dynamics (MD) simulations in explicit solvent. We also investigate the influence of head-group size, using HEA^+, HBA^+, HPA^+ The twelve systems were simulated for 200ns each. Computational simulations were performed using GROMOS 54a7 [3] force field and GROMACS program [4]. The results show that formation of the molecular aggregates is depend of the chemical nature of counterions, as can been seen in figure 1. Also, was observed that head-group size affect the shape of micelle. Details about protocols and others structural results will be presented and discussed during the conference.



HEAF HEACl HEABr HEAI

Figure 1: Structures of micelles after 200ns .

Key-words: **Surfactants, Counterions, Molecular Dynamics**……..
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