# Mesophase behavior of Cetyltrimethylammonium chloride: insights from all-atom Molecular Dynamics simulations

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CetylTrimethylAmmonium Chloride (CTAC) with chemical formula $C_{19}H_{42}ClN$ belongs to the family of Alkytrimethilamomonium chlorides (ATACs) which are common cationic surfactants with applications as antiseptics, conditioners and other recipes of health and personal care products. CTAC aqueous solutions exhibit a rich phase behavior over a range of concentrations and temperatures as observed experimentally.[1] As a complementary approach, molecular modelling has been used extensively to predict the structural, thermodynamic and transport properties of surfactant solutions. Nevertheless, to the best of our knowledge, the morphology for higher surfactant concentrations, has been studied with all-atom (AA) models utilizing pre-assembled initial configurations based on the experimental observation for the thermodynamic states of interest; alternatively, coarse grain models have been able to predict the morphology of surfactant systems notwithstanding the lack of important details in the atomistic level. [2]

In this work, we explore the phase diagram of CTAC aqueous solutions for relatively high concentration by means of all-atom molecular dynamics (AA-MD) simulations. For the first time, by applying a specific simulation protocol and starting from random initial configurations, a plethora of different phases were identified, in agreement with the experimental findings for a range of concentrations from 34 wt % up to 87 wt %; from lower to higher concentration the system exhibits micellar, hexagonal, intermediate and lamellar phase. These phases were analyzed using an in-house developed algorithm [3] providing details not only on the solvation environment, the shape and dimensions of CTAC assemblies but also on the molecular mechanisms of the observed phases transformations. Our methodology paves the way for the investigation of phase behavior for other ATACs that is still on debate.

References:

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