Comparison of the Effect of Poly (N-vinyl caprolactam) and Poly (N-isopropyl acrylamide) trimers on the Stability of Hydrated Na-montmorillonite: A Molecular Dynamics Study

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In the present study, we performed a molecular dynamics (MD) simulation of the intercalation of poly (N-vinyl acrylamide) $(NIPAM)_3$ and poly (N-vinyl caprolactam) $(NVCL)_3$ trimers into Na-montmorillonite (Na-Mt) to evaluate their effect on the interlayer structure and the stability of hydrated Na-Mt.

The impact of both trimers on the interlayer species and their dynamics properties at 300, 305. 315, 325K in a canonical ensemble (NVT) were investigated. Material Studio 7.0 software under the module "Forcite", Universal Force Field (UFF), SPC/E water model, and CVFF Forcefields for both polymers were employed with 800 water molecules in 32-unit cell of Na-Mt.

The results showed that the electrostatic forces exerted by Na cations on H_2O molecules and the interlayer H_2O molecules arrangement are not affected by the rise in temperature after adding the trimers. Trimers addition reinforced the structure of interlayer H_2O molecules so that the effect of temperature increase on them became negligible. The structural dynamics evolution of the radius of gyration of both trimers showed the existence of small change in the conformation near 305 K and these conformational changes are more complex in the case of $(NVCL)_3$ than $(NIPAM)_3$ due to its large monomers which affected its intrinsic viscosity. Both trimers reduced the mobility of interlayer particles with a better inhibition effect obtained for $(NVCL)_3$ compared to $(NIPAM)_3$. The concentration profile of interlayers species showed the affinity of Na cations for clay mineral surfaces while H_2O molecules moved away.

Compared these two trimers, the most stable state of Na-Mt is achieved with $(NVCL)_3$. These results could help highlight the inhibition properties of $(NVCL)_3$ and $(NIPAM)_3$ on hydrated Na-Mt and to predict its stability against environmental condition changes.

Key words: Na-Mt, oligomer, Thermosensitive polymers, Molecular dynamics, Radial distribution function, Self-diffusion coefficient, Radius of gyration, Intrinsic viscosity, Concentration profile.