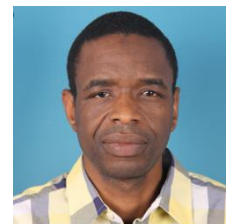


## Comparison of the Effect of Poly (N-vinyl Caprolactam) and Poly (Nisopropyl Acrylamide) trimers on the Stability of Hydrated Namontmorillonite: A Molecular Dynamics Study



Moussa Camara, Hualin Liao, Jiafang Xu, Jun Zhang  
China University of Petroleum, China

### Abstract

In the present study, we performed a molecular dynamics (MD) simulation of the intercalation of poly (N-isopropyl acrylamide) (NIPAM)<sub>3</sub> and poly (N-vinyl caprolactam) (NVCL)<sub>3</sub> 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 different temperature in a canonical ensemble (NVT) were investigated. The results showed that the electrostatic forces exerted by Na cations on H<sub>2</sub>O molecules and the interlayer H<sub>2</sub>O molecules arrangement are not affected by the rise in temperature after adding both trimers. Trimers addition reinforced the structure of interlayer H<sub>2</sub>O 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 conformation changes when temperature increased. These conformational changes are more complex in the case of (NVCL)<sub>3</sub> than (NIPAM)<sub>3</sub> due to its large monomers. Both trimers reduced the mobility of interlayer particles with a better inhibition effect obtained for (NVCL)<sub>3</sub> compared to (NIPAM)<sub>3</sub>. The concentration profile of interlayer's species showed the affinity of Na cations for clay mineral surfaces while H<sub>2</sub>O molecules moved away. Compared these two trimers, the most stable state of Na-Mt is achieved with (NVCL)<sub>3</sub>. These results could help highlight the inhibition properties of (NIPAM)<sub>3</sub> and (NVCL)<sub>3</sub> on hydrated Na-Mt and to predict its stability against environmental condition changes.



**Biography:** Moussa Camara is well-known author in the field of Clay and Clay Minerals, Clay Polymer Nanocomposites and Drilling and Completion Fluids Chemistry for over 6 years in the department of Oil & Gas Well Engineering at China University of Petroleum (East China). He is working now on the rheological properties of thermosensitive polymers in water based drilling fluids, and clay swelling inhibitors using Molecular Dynamics Simulation methods.

### Speaker Publications:

1. "Molecular dynamics simulation of hydrated Namontmorillonite with inorganic salts addition at high temperature and high pressure" *Applied Clay Science*/2017/ 146:206-215.
2. "Molecular Dynamics Study of the Intercalation and Conformational Transition of Poly (N-vinyl Caprolactam), a Thermosensitive Polymer in Hydrated Na-montmorillonite" *Polymer*/2019/ 179:121718
3. "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." *Polymers and Polymer Composites*/2020.

[7<sup>th</sup> world congress on Chemical Engineering and Catalysis 2020](#) Webinar– July 22-23, 2020.

**Abstract Citation:**

Moussa Camara, Comparison of the Effect of Poly (N-vinyl Caprolactam) and Poly (Nisopropyl Acrylamide) trimers on the Stability of Hydrated Namontmorillonite: A Molecular Dynamics Study, Chemical Engineering Congress 2020, 7<sup>th</sup> World Congress on Chemical Engineering and Catalysis Webinar- July 22-23,2020

(<https://chemicalengineering.annualcongress.com/abstract/2020/comparison-of-the-effect-of-poly-n-vinyl-caprolactam-and-poly-nisopropyl-acrylamide-trimers-on-the-stability-of-hydrated-namontmorillonite-a-molecular-dynamics-study>)