# Molecular dynamic simulations of kaolinite intercalation by dimethylformamide

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**Abstract**: Molecular dynamic simulations of kaolinite-dimethylformamide complex models with increasing numbers of dimethylformamide molecules in the interlayer space were performed. It was found that the basal spacing of kaolinite can be considerably enlarged by the intercalation of small organic molecules with the prerequisite of overcoming the intercalation energy barrier. Based on the computation of interfacial structure and interaction of the model that produced the basal spacing of 1.26 nm, it was found that the dimethylformamide was arranged as monolayer structure in the interlayer space. The molecular plane of dimethylformamide oriented at the angle of around 60° with respect to the interlayer surface with the oxygen atom of HC=O group functioned as proton acceptor forming strong H-bonds with the hydroxyl group on the interlayer octahedral surface. The methyl group of dimethylformamide bonded to the tetrahedral surface through hydrophobic interaction. The octahedral surface possessing highly active surface hydroxyl groups showed stronger bonding affinity toward the dimethylformamide compared to the tetrahedral surface.

**Keywords**: Kaolinite; Dimethylformamide; Intercalation; Molecular dynamics simulation