*Supplementary Information for*

**Molecular dynamics simulation of dodecyl dimethyl benzyl ammonium (DDBA) intercalated-****montmorillonite**

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This file includes Tables S1 and calculation details of the density of the organic phase formed by the lauryl chains

**1. MSDs of interlayer dodecyl dimethyl benzyl ammonium (DDBA) in DDBA-Mnt systems**



**Fig. S1.** The mean squared displacement (MSD) of interlayer dodecyl dimethyl benzyl ammonium (DDBA) in DDBA-Mnt systems (N\*: N atoms of DDBA that were not attached to the clay mineral surface). a: DA-6 system; b: DA-13 system; c: DA-24 system; d: DA-34 system.

**2. Calculation details of the density of the organic phase formed by the lauryl chains**

The density of the organic phase formed by the lauryl chains is calculated as follows (Liu *et al*., 2007):

$$D=M/(S×\left(b-h×2\right))$$

where M denotes the mass of the lauryl chains, S is the area of the basal surface, b is the basal spacing and h is the average distance of the organic phase from the clay surface. h is taken as 3.5 Å, 2.4 Å, 2.5 Å and 2.6 Å in DA-6, DA-13, DA-24 and DA-34, respectively, based on the density profiles (Fig. 2) where it can be observed that the lauryl chains in all systems are limited in the spaces ~ h+6.64 Å (clay sheet is 6.64 Å thick) from the (z = 0) plane.

**References**

Liu, X.D**.**, Lu, X.C., Wang, R.C., Zhou, H.Q. & Xu, S.J. (2007) Interlayer Structure and Dynamics of Alkylammonium-intercalated Smectites with and without Water: A Molecular Dynamics Study. *Clays and Clay Minerals,* **55***,* 554-564.