Electronic Supplementary Information (ESI) for

Understanding the Thermal Motion of the Luminescent Dyes in the Dye-Surfactant Cointercalated ZnAl-Layered Double Hydroxides: a Molecular Dynamic Study

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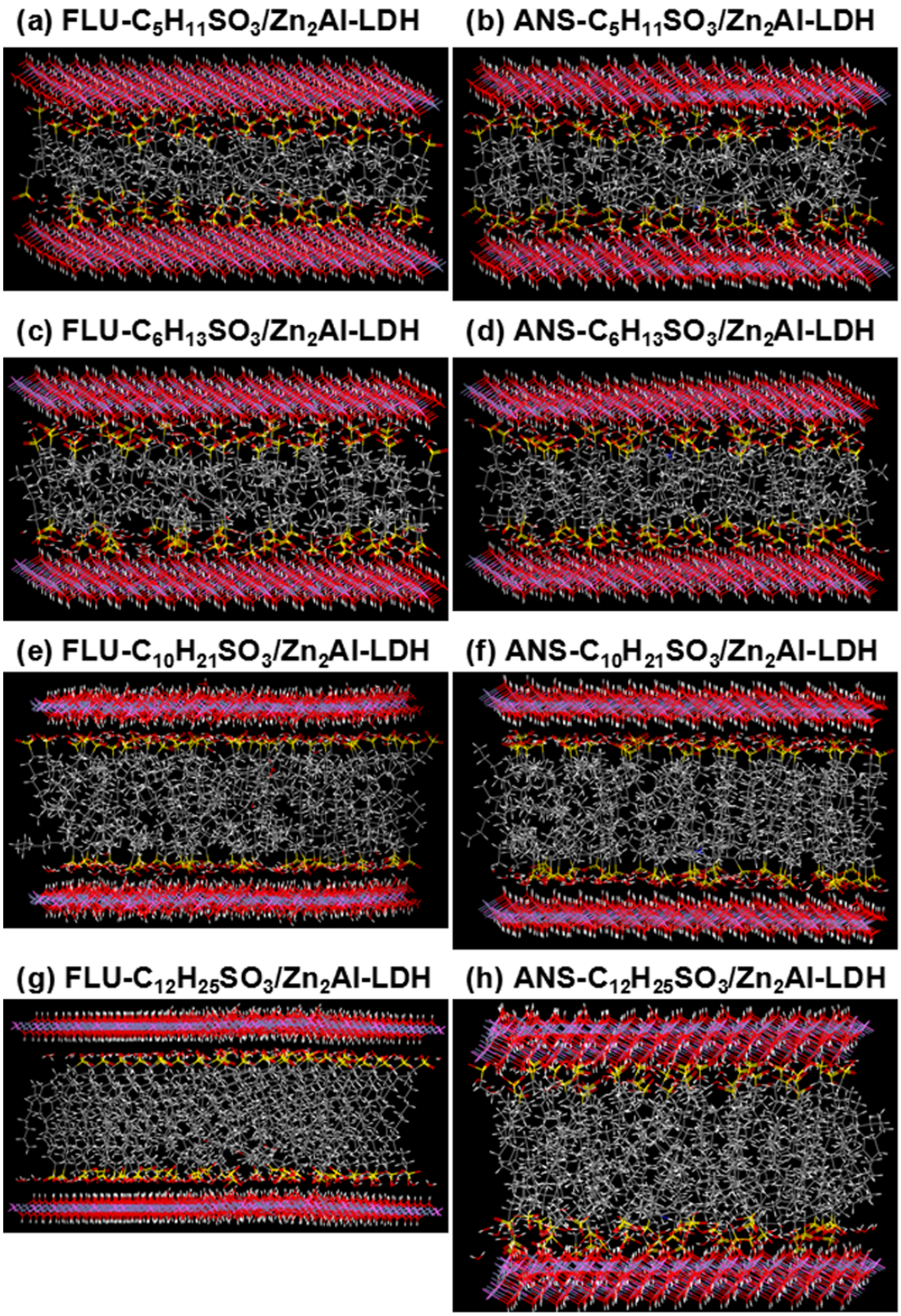

Fig. S1 The snapshots of dye-$C_nH_{2n+1}SO_3/Zn_2Al$-LDH (n = 5, 6, 10 or 12, respectively) after molecular dynamics simulations of 10 ns.

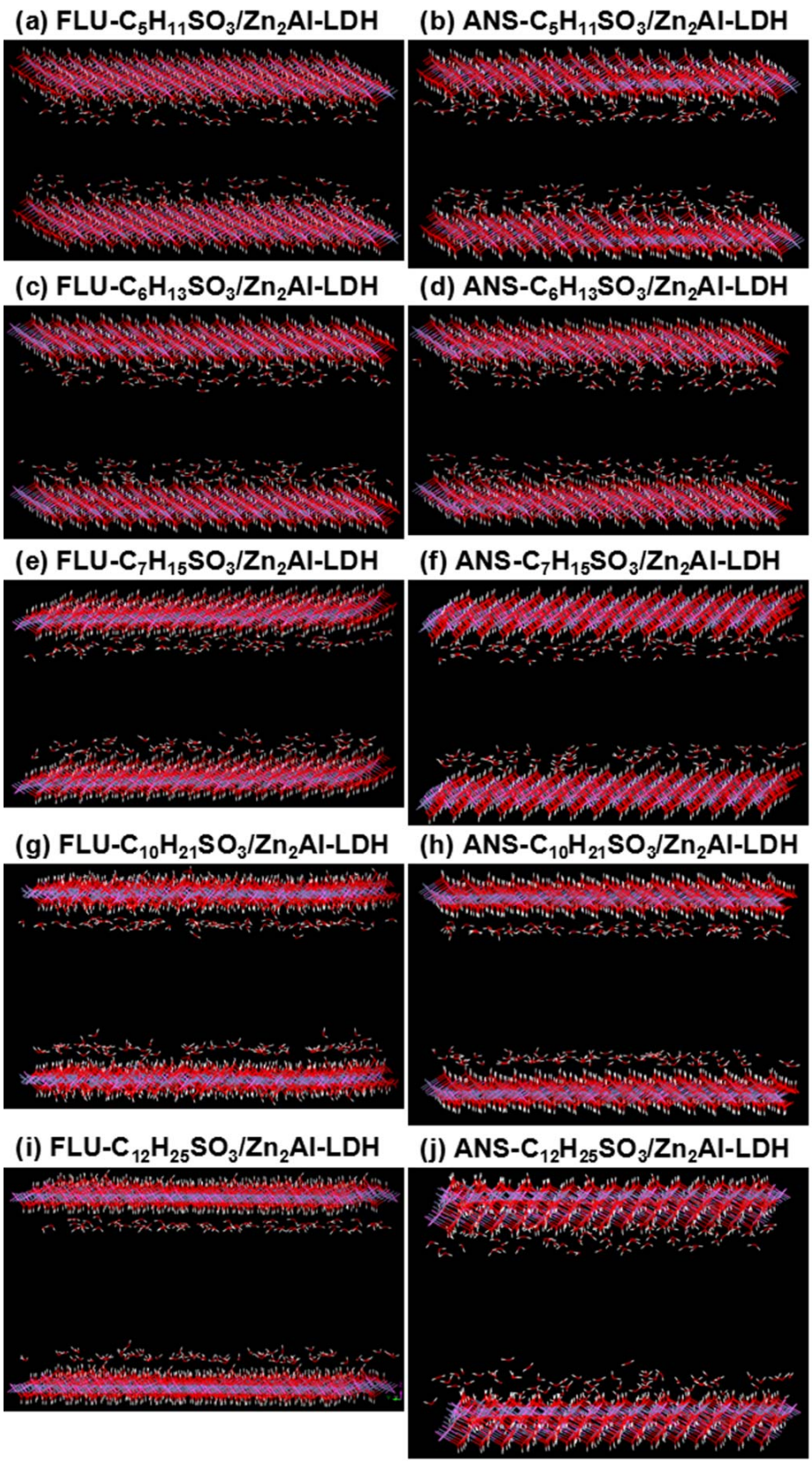

Fig. S2 The snapshots of dye-$C_nH_{2n+1}SO_3$/Zn_2Al-LDH (n = 5, 6, 7, 10 or 12, respectively) after molecular dynamics simulations of 10 ns with dye and $C_nH_{2n+1}SO_3$ omitted.

Table S1 Detailed E_{model}, E_{dye} and $E_{model\ without\ dye}$ of LDHs-based models.

Model	E_{model} / kcal•mol^{-1}	E_{dye} / kcal•mol^{-1}	$E_{model\ without\ dye}$ / kcal•mol^{-1}
FLU-$C_5H_{11}SO_3$/Zn_2Al-LDH	-257509.90	26.32	-257399.28
FLU-$C_6H_{13}SO_3$/Zn_2Al-LDH	-256069.82	26.32	-255955.01
FLU-$C_7H_{15}SO_3$/Zn_2Al-LDH	-257636.24	26.32	-257359.25
FLU-$C_{10}H_{21}SO_3$/Zn_2Al-LDH	-264251.29	26.32	-264077.06
FLU-$C_{12}H_{25}SO_3$/Zn_2Al-LDH	-256821.47	26.32	-256724.28
ANS-$C_5H_{11}SO_3$/Zn_2Al-LDH	-254474.43	119.99	-254435.67
ANS-$C_6H_{13}SO_3$/Zn_2Al-LDH	-254587.85	119.99	-254536.04
ANS-$C_7H_{15}SO_3$/Zn_2Al-LDH	-257565.24	119.99	-257497.07
ANS-$C_{10}H_{21}SO_3$/Zn_2Al-LDH	-254695.84	119.99	-254682.38
ANS-$C_{12}H_{25}SO_3$/Zn_2Al-LDH	-256635.89	119.99	-256651.16
FLU-HPS/$Zn_{0.827}Al_{0.173}$-LDH	-266855.26	26.32	-266747.23
FLU-HPS/$Zn_{0.787}Al_{0.213}$-LDH	-263953.36	26.32	-263760.55
FLU-HPS/$Zn_{0.747}Al_{0.253}$-LDH	-263549.68	26.32	-263318.06
FLU-HPS/$Zn_{0.707}Al_{0.293}$-LDH	-257530.51	26.32	-257291.90
ANS-HPS/$Zn_{0.827}Al_{0.173}$-LDH	-269322.64	119.99	-269406.20
ANS-HPS/$Zn_{0.787}Al_{0.213}$-LDH	-266425.78	119.99	-266466.42
ANS-HPS/$Zn_{0.747}Al_{0.253}$-LDH	-263524.30	119.99	-263512.08
ANS-HPS/$Zn_{0.707}Al_{0.293}$-LDH	-260411.97	119.99	-260358.01

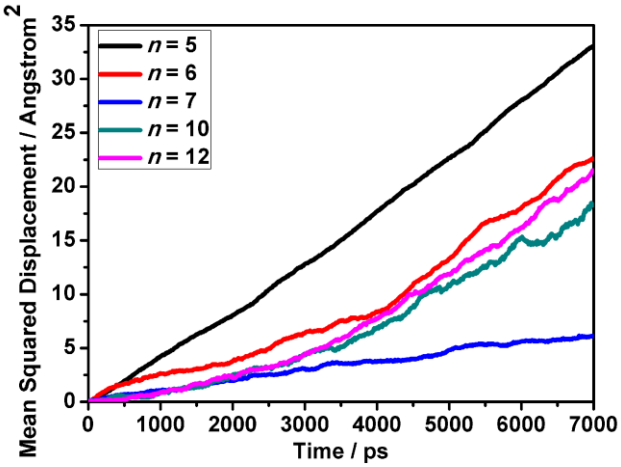

Fig. S3 The plots of mean squared displacement as the function of time for FLU-$C_nH_{2n+1}SO_3/Zn_2Al$-LDHs.

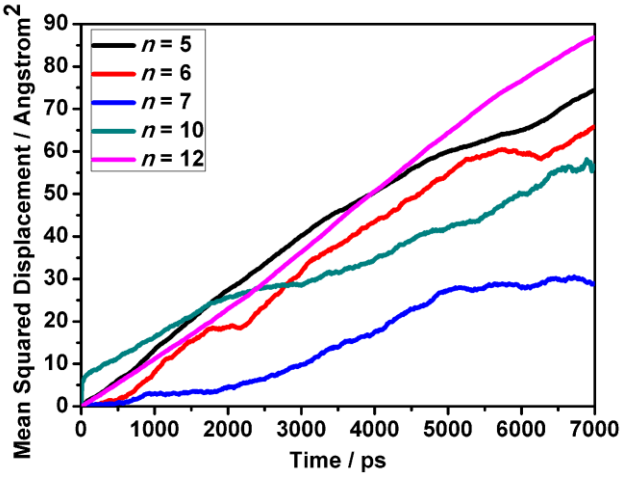

Fig. S4 The plots of mean squared displacement as the function of time for ANS-$C_nH_{2n+1}SO_3/Zn_2Al$-LDHs.

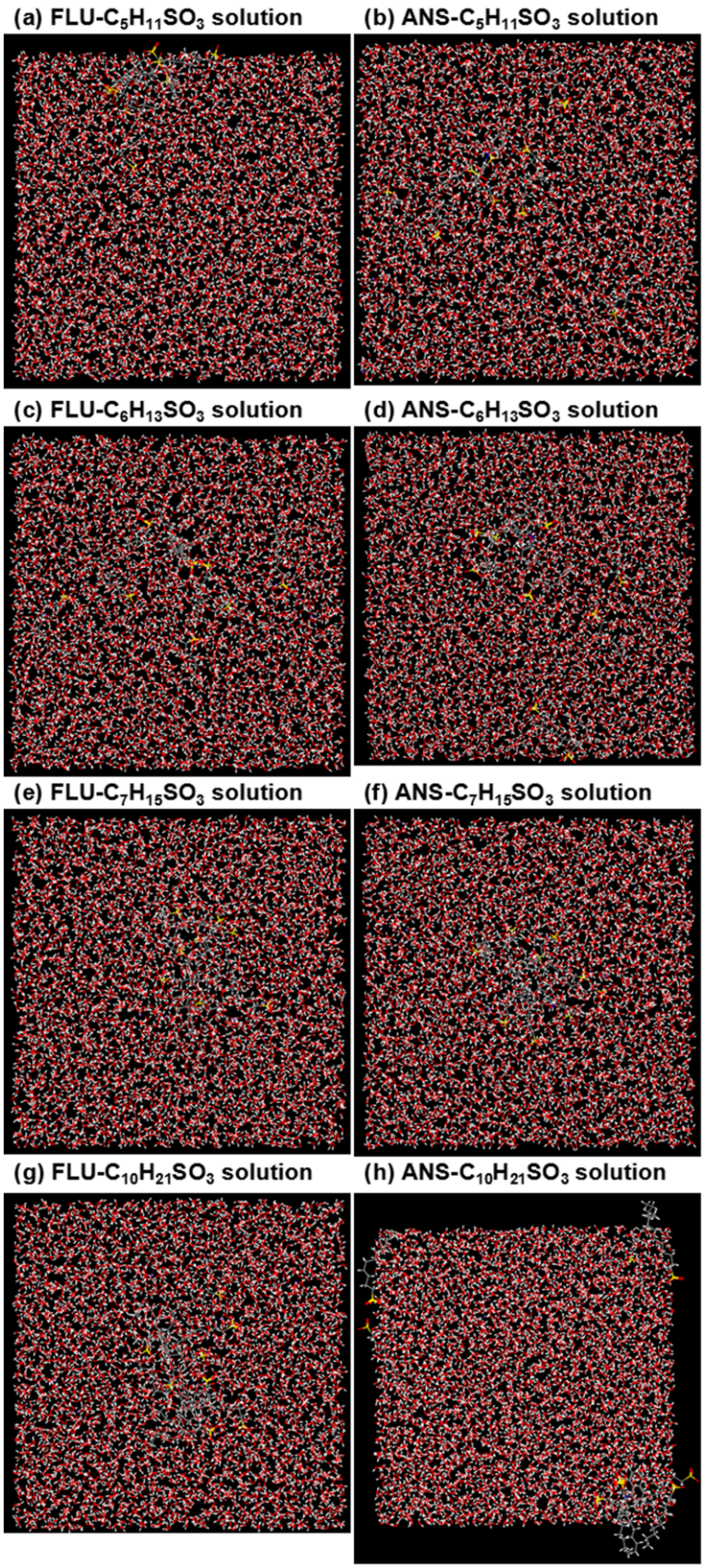

Fig. S5 The snapshots of dye-$C_nH_{2n+1}SO_3$ solution (n = 5, 6, 7 and 10, respectively) after molecular dynamics simulations of 10 ns.

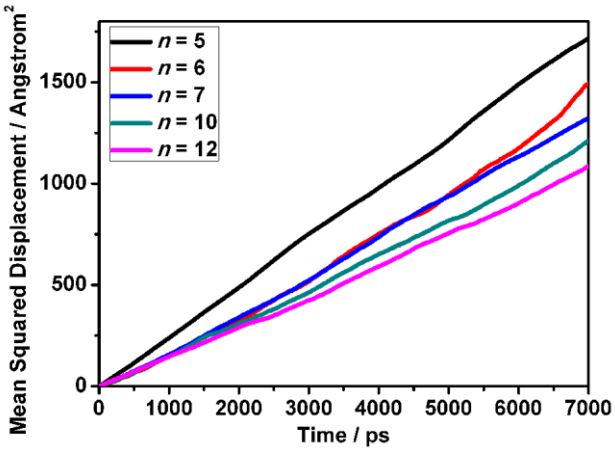

Fig. S6 The plots of mean squared displacement as the function of time for FLU-$C_nH_{2n+1}SO_3$ solutions (n = 5, 6, 7, 10 and 12, respectively).

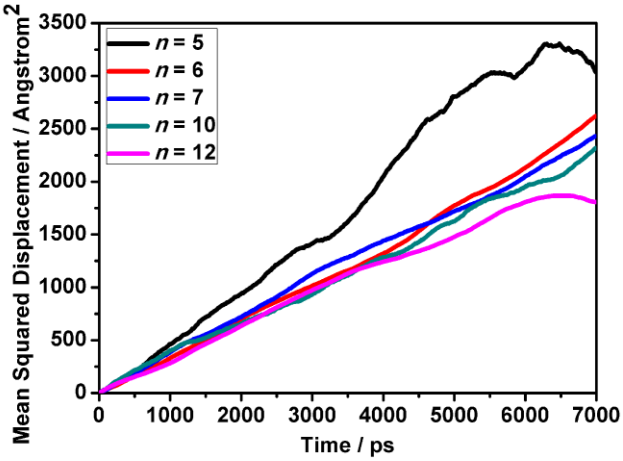

Fig. S7 The plots of mean squared displacement as the function of time for ANS-$C_nH_{2n+1}SO_3$ solutions (n = 5, 6, 7, 10 and 12, respectively).

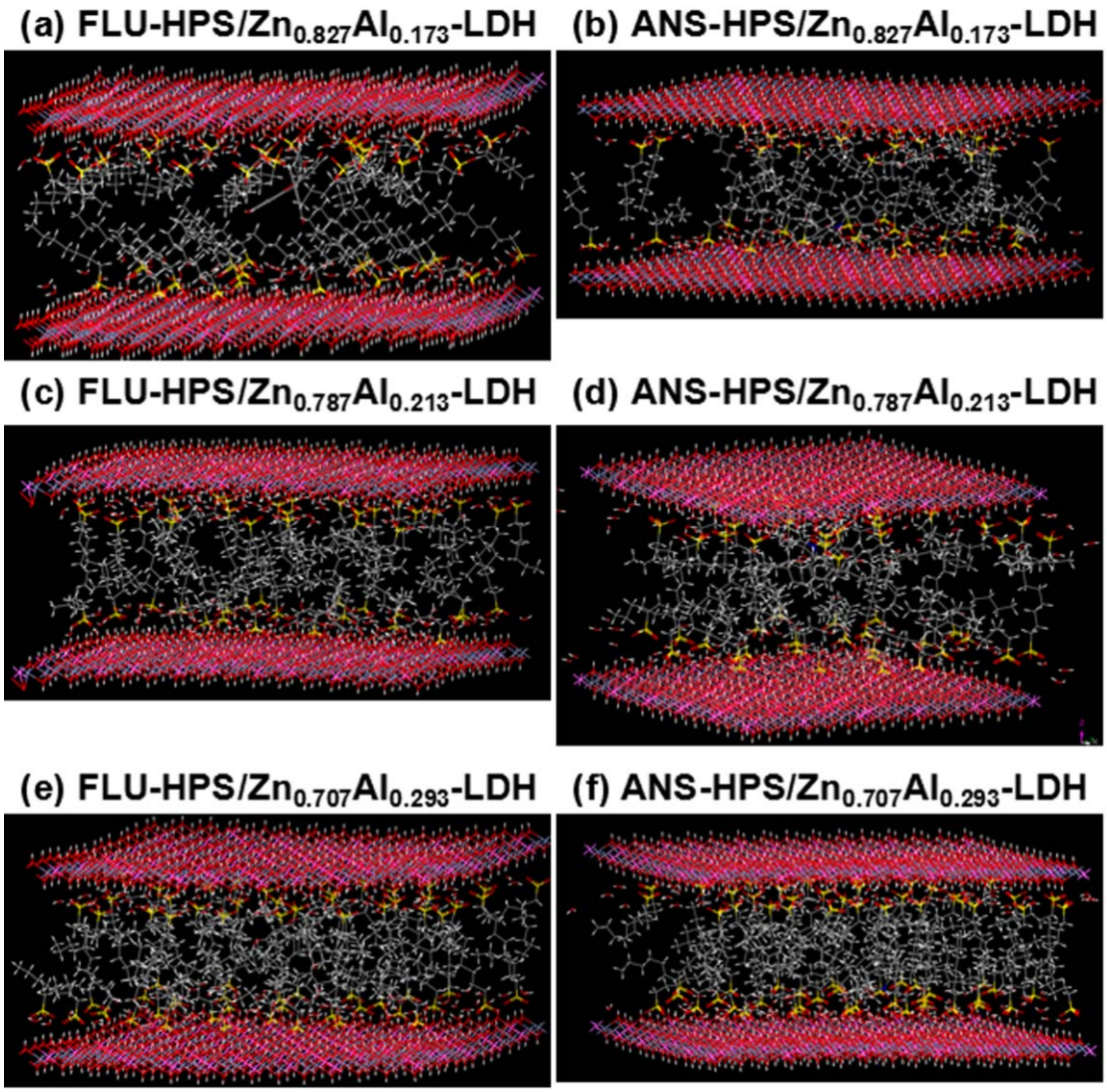

Fig. S8 The snapshots of dye-HPS/$Zn_{1-x}Al_x$-LDHs (x = 0.173, 0.213 and 0.293, respectively) after molecular dynamics simulations of 10 ns.

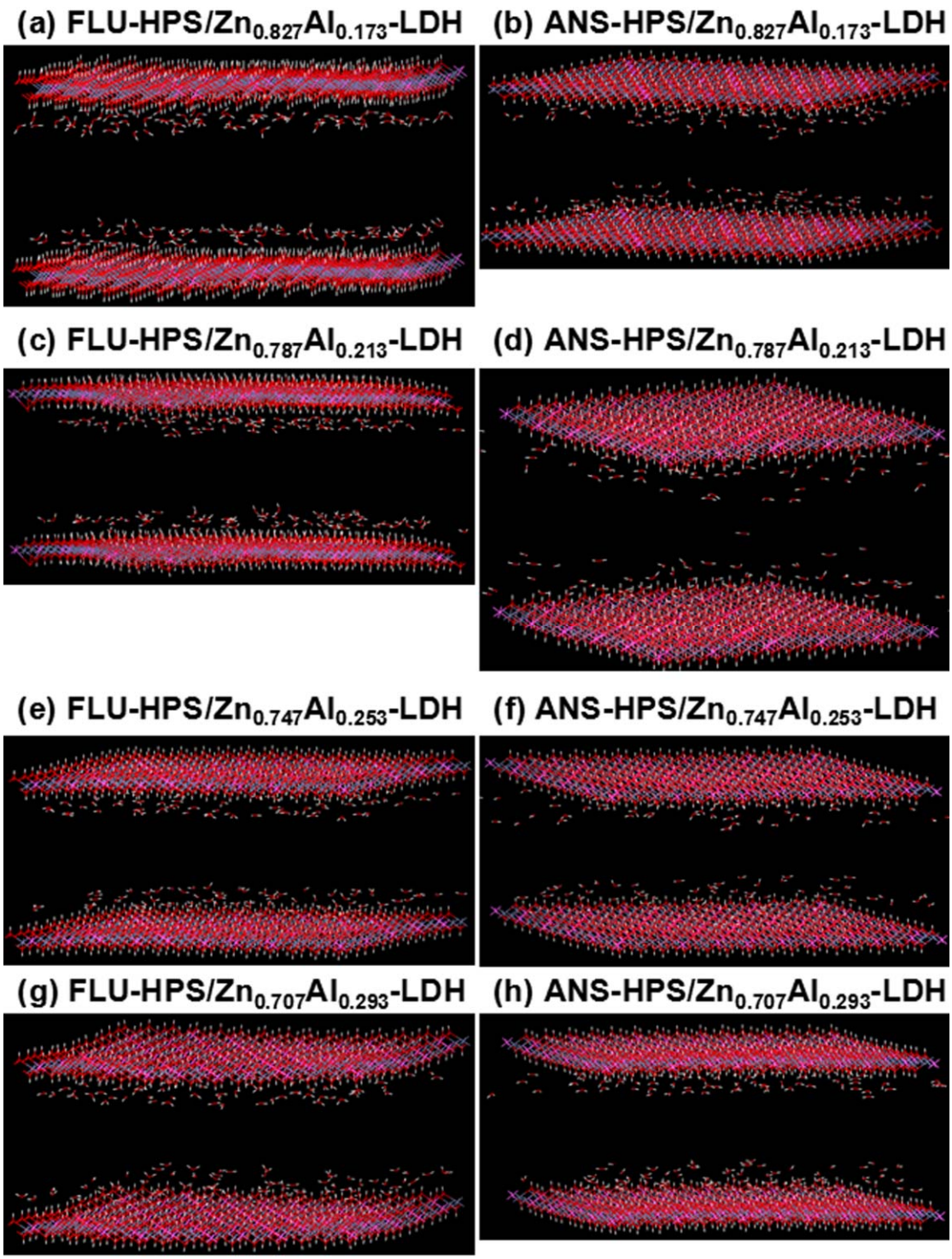

Fig. S9 The snapshots of dye-HPS/$Zn_{1-x}Al_x$-LDHs (x = 0.173, 0.213, 0.253 and 0.293, respectively) after molecular dynamics simulations of 10 ns with dye and HPS omitted.

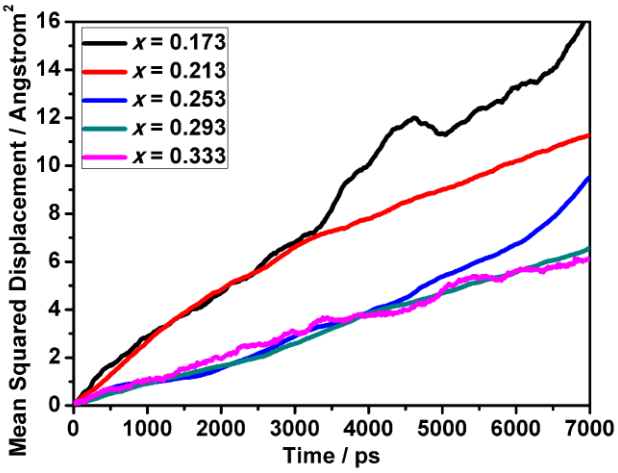

Fig. S10 The plots of mean squared displacement as the function of time for FLU-HPS/$Zn_{1-x}Al_x$-LDHs.

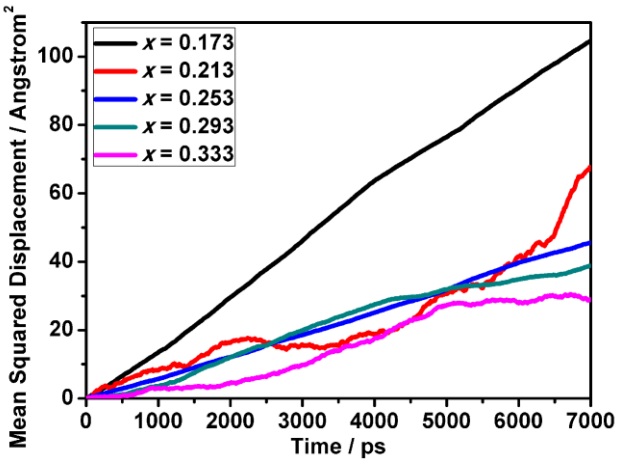

Fig. S11 The plots of mean squared displacement as the function of time for ANS-HPS/$Zn_{1-x}Al_x$-LDHs.