Electronic Supplementary Information

Molecular Design Confirmation for Proposition of Improved Photophysical Properties in a Dye-Intercalated Layered Double Hydroxides

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Fig. S1. Time profiles of the total energy (the last 2000 ps)

Fig. S 2.EDX images of Red 27- Zn-Al-LDH

Fig. S3. Photogram of a: Emission wavelength of the Red 27-Zn_2Al-LDH at436nm, b: Emission wavelength of the Red 27-Zn_2Al-LDH at542nm, c:Emission wavelength of the Acid Red 27 at 440nm, and d:Emission wavelength of the Acid Red 27 at 569nm.

Fig. S4. H type (face to face) arrangement and coplanar conformation of the Acid Red 27 molecules with π- π interaction which is presented by the molecular dynamic simulation.

Fig. S5. Distribution of the tilt angle (θ) of the tail vectors of the Red 27 molecules with respect to normal to the interface

Fig. S6. RDFs between the endgroup of Acid Red 27 and the water molecules in the LDH system

Fig. S7. Hydrogen bonds in the hybrid system and the angle between the tail vector of the Acid Acid Red 27 molecules and the layer surface

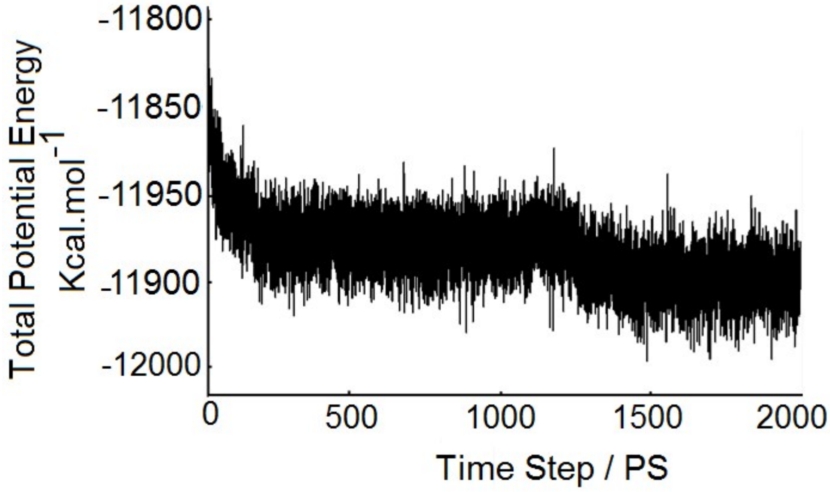

Fig.S1 Time profiles of the total energy (the last 2000 ps)

Fig. S1 shows that the potential energy profile reaches stable equilibrium after about 1000ps of simulation time and last 2000 ps was used for further analysis.

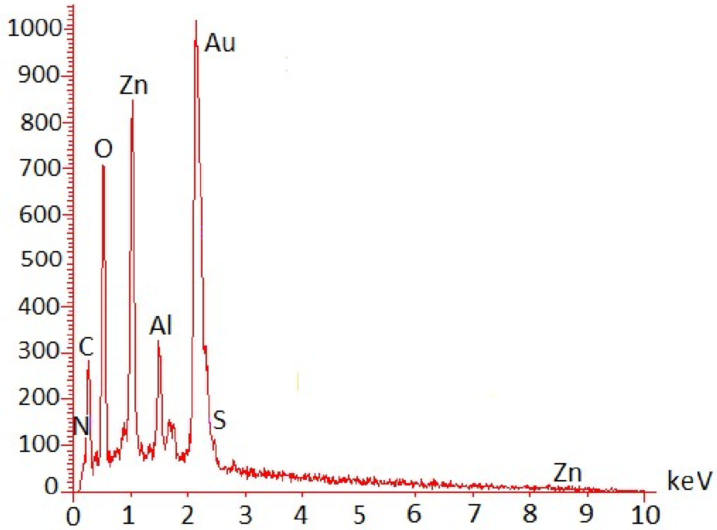

Fig.S 2.EDX images of Red 27- Zn-Al-LDH

Fig. S2 The chemical composition of Al, Zn, O, C, N, and S in the Red 27- Zn-Al-LDH nanohybride at the microscopic level was analyzed by the energy dispersive X-ray spectroscopy (EDX)

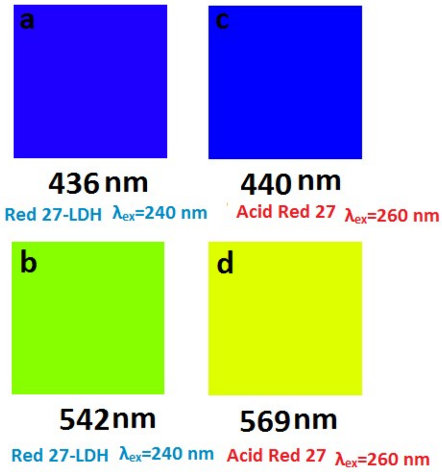

Fig.S3 Photogram of a: Emission wavelength of the Red 27-Zn_2Al-LDH at436nm, b: Emission wavelength of the Red 27-Zn_2Al-LDH at542nm, c:Emission wavelength of the Acid Red 27 at 440nm, and d:Emission wavelength of the Acid Red 27 at 569nm.

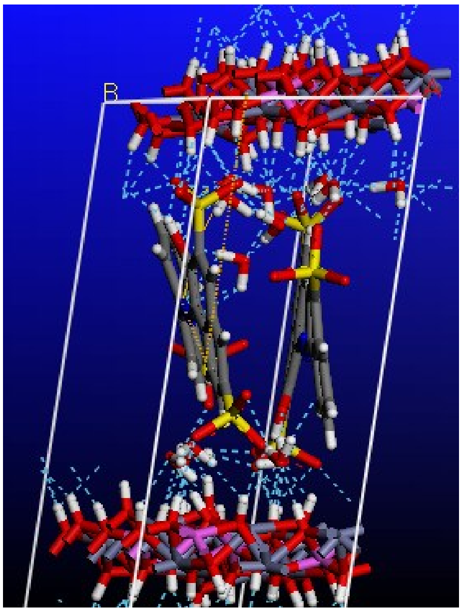

Fig.S4H type (face to face) arrangement and coplanar conformation of the Acid Red 27 molecules with π- π interaction which is presented by the molecular dynamic simulation.

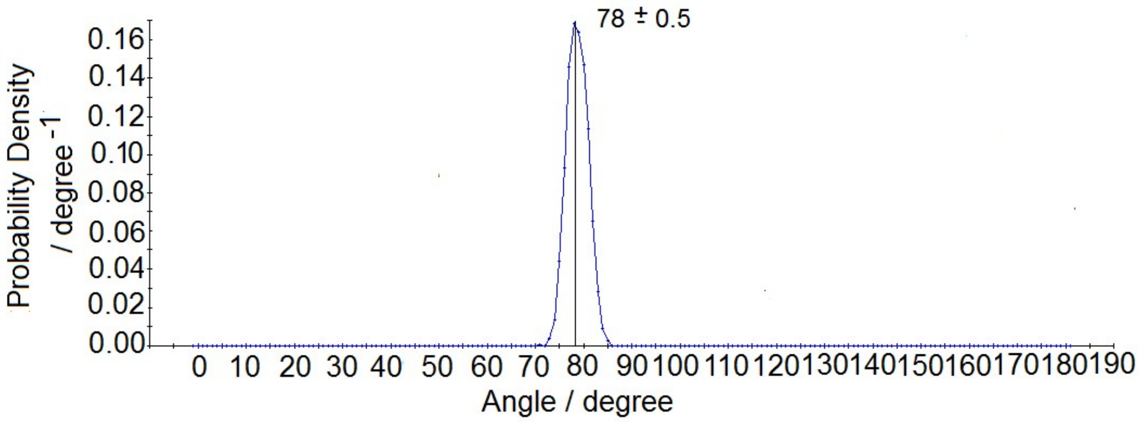

Fig. S5 Distribution of the tilt angle (θ) of the tail vectors of the Red 27 molecules with respect to normal to the interface

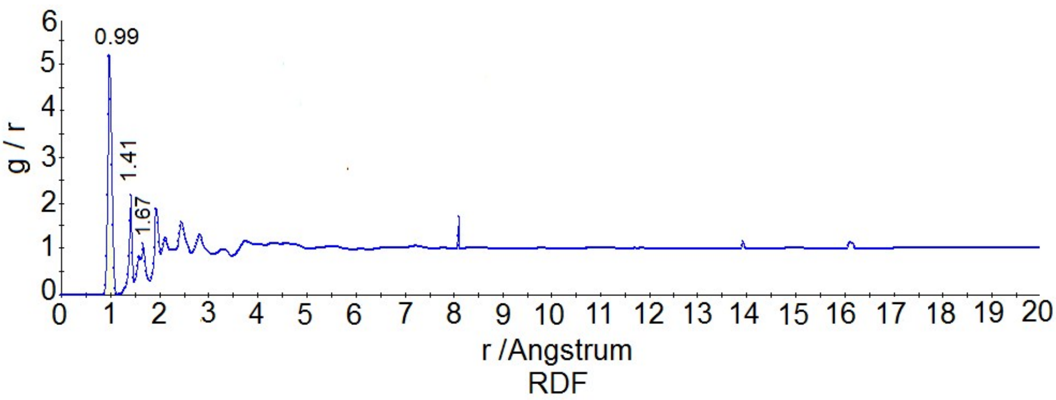

Fig.S6RDFs between the endgroup of Acid Red 27 and the water molecules in the LDH system

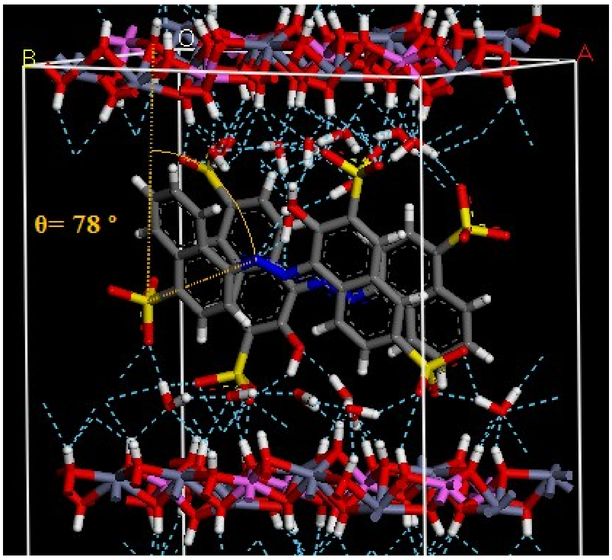

Fig.S7 Hydrogen bonds in the hybrid system and the angle between the tail vector of the Acid Acid Red 27 molecules and the layer surface