Electronic Supplementary information for

A Combined Study based on Experiment and Molecular Dynamics: Perylene Tetracarboxylate Intercalated in Layered Double Hydroxide Matrix

Dongpeng Yan, Jun Lu, * Min Wei, * Jing Ma, David G. Evans, and Xue Duan

State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing 100029, P. R. China, and School of chemistry and chemical engineering, Key Laboratory of Mesoscopic Chemistry of MOE, Nanjing University, Nanjing 210093, P.R. China

Details of the forcefield parameters for MD simulation of Mg-Al-LDH:

The equilibrium bond length parameter of Mg–O was adopted from the modified Dreiding forcefield,[1] i.e., r_0 = 2.100Å, and other forcefield parameters in Eq 1, k_i (i=2, 3, 4), were assigned the same parameters as Al atoms in modified cff91 forcefield.[2]

$$E=k_2(r - r_0)^2 + k_3(r - r_0)^3 + k_4(r - r_0)^4 \quad (1)$$

The bond angle parameters of Mg–O–Mg or O–Mg–O, k_i' (i = 2, 3, 4) and θ_0 = in Eq 2, were also the same as those of Al atoms in modified cff91 forcefield,[2] and similar treatment were also observed in the Newman *et al*'s work.[1]

$$E=k_2'(\theta - \theta_0)^2 + k_3'(\theta - \theta_0)^3 + k_4'(\theta - \theta_0)^4 \quad (2)$$

The ε value in Lennard-Jones (LJ) 9-6 potential parameters (Eq 3) of Mg was assigned the same as that of Al atoms based on the Li et al's work,[2] and the r^0 value was determined by non-linear fitting method based on the consistent-valence forcefield (CVFF) given by Kim *et al*,[3] and ε =1.5767 kcal/ mol, r^0 = 2.4587 Å.

$$E=\varepsilon[2\times(\frac{r^0}{r})^9-3\times(\frac{r^0}{r})^6] \quad (3)$$

To further test the discrepancy of properties of LDH influenced by the forcefield parameters, we simulate the model of $Mg_{12}Al_6(OH)_{32}(CO_3)_2\cdot 8H_2O$, and the above forcefield parameters were used, all the simulation condition was the same as that in the main text. The calculated average interlayer spacing was 7.69 Å, which is very close to Aicken's computational result,[4] and is also consistent with the experiment one (7.65 Å), demonstrating the precision of this modified

forcefield for Mg-Al-LDH.

[1] S. P. Newman, T. D. Cristina, P. V. Coveney, W. Jones, *Langmuir* 2002, **18,** 2933.

[2] H. Li, J. Ma, D. G. Evans, T. Zhou, F. Li, X. Duan, *Chem. Mater*. 2006, **18,** 4405.

[3] N. Kim,; A. Harale, T. T. Tsotsis, M. Sahimi, *J. Chem. Phys.* 2007, **122**, 224701.

[4] A. M. Aicken, I. S. Bell, P. V. Coveney, W. Jones, *Adv. Mater*. 1997, **9,** 496.

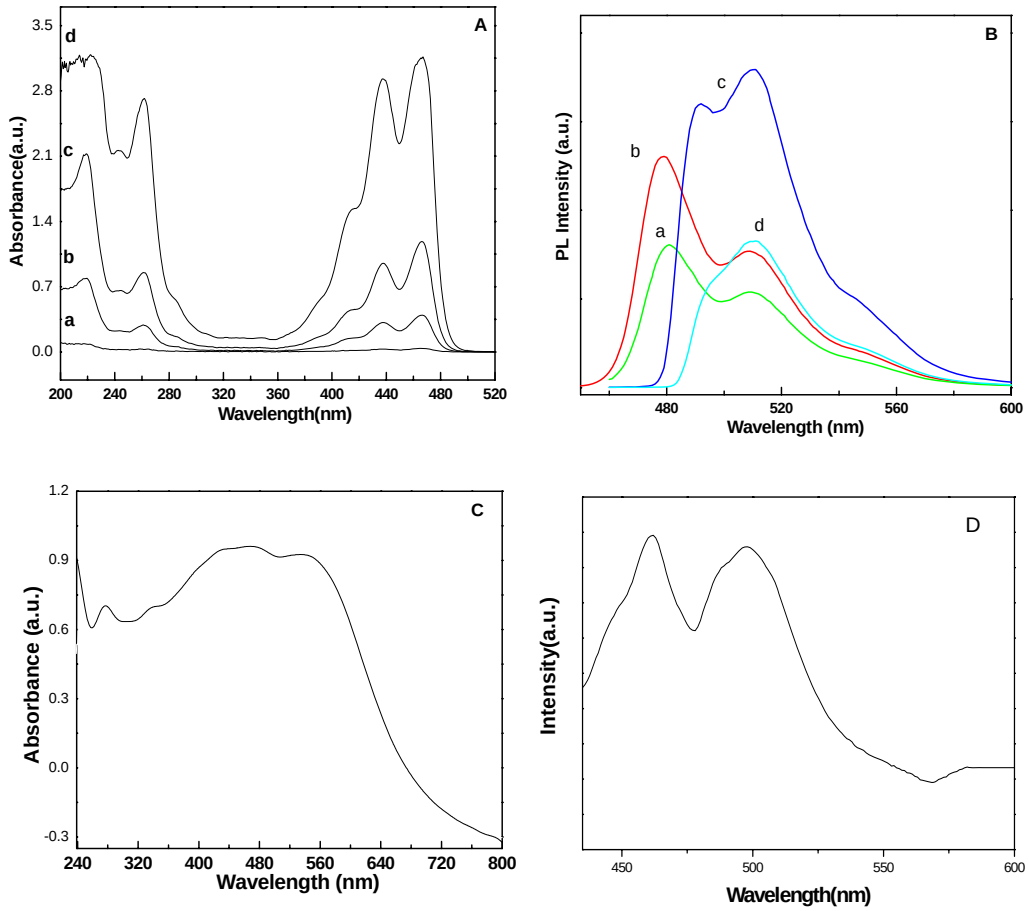

Figure S1. (A) UV-vis absorption spectra and (B) photoluminescence spectra of PTCB aqueous solution with various concentrations: (a) 1 μM, (b) 3 μM, (c) 10 μM and (d) 30 μM. (C) UV-Vis absorption spectra and (D) photoemission spectra of PTCB/LDH powder.

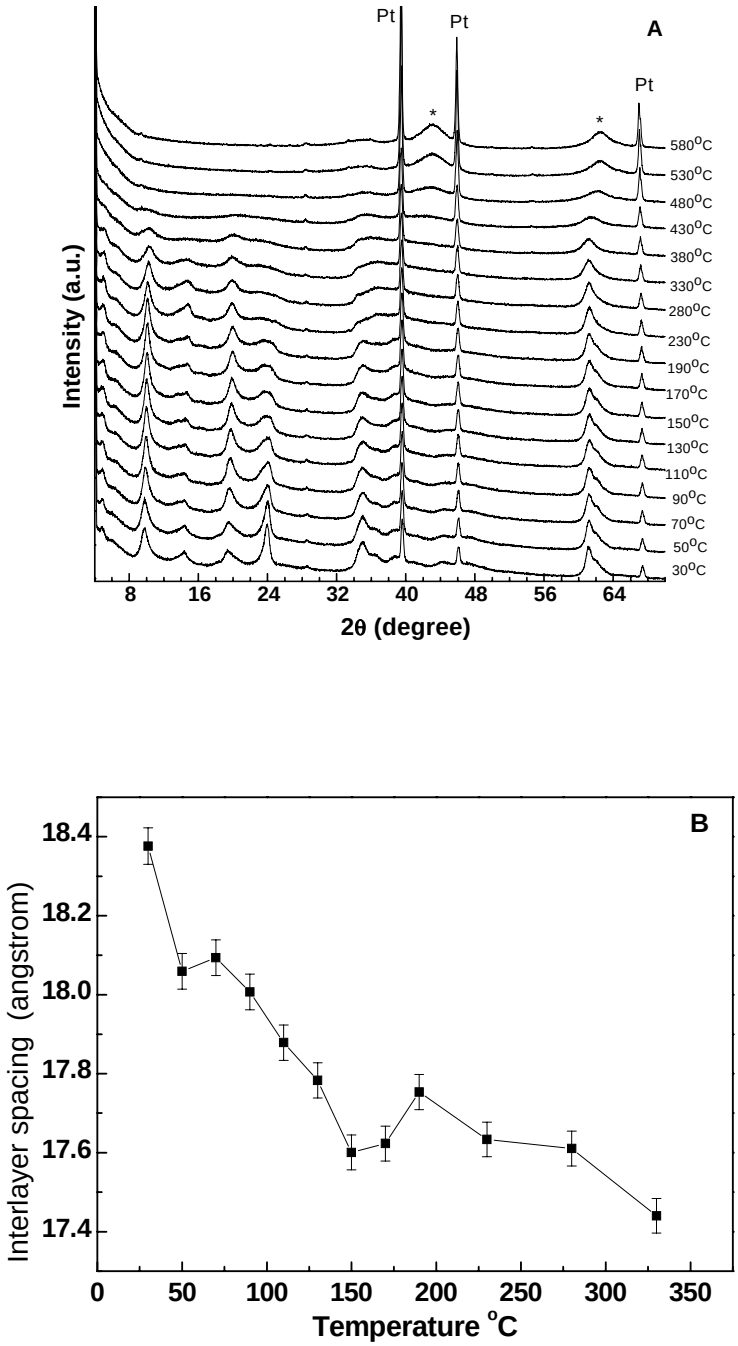

Figure S2 *In situ* XRD patterns of PTCB intercalated Mg-Al-LDH in the temperature range 30-580 °C: (A) 2θ angular domain from 4 to 70° (*: MgO); (B) Variation of the interlayer spacing with temperature.

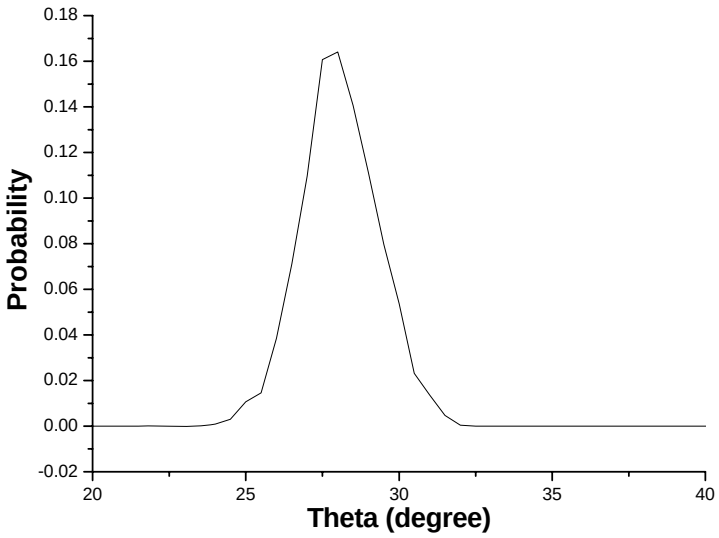

Figure S3. The distribution of the orientation angle of PTCB under the experimental hydration states.