Support information

Revealing the Mechanism of Glutamic Acid-Functionalized Layered Double Hydroxides and its Removal Mechanism for Cr(VI) from Microscopic and Macroscopic Perspectives

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1 Experimental

1.1 Chemicals

Glutamic acid, Iron nitrate nonahydrate ($Fe(NO_3)_3·9H_2O$), Potassium Chromate (K_2CrO_4), Nickel nitrate hexahydrate ($Ni(NO_3)_2·6H_2O$), urea (CH_4N_2O), and ammonium fluoride (NH_4F) were obtained from Sinopharm Chemical Reagent Co. Ltd., China. Hydrochloric acid (HCl), Potassium hydroxide (KOH), Absolute ethanol, and Nitric acid (HNO_3) were supplied by Shanghai Xilong Chemical Co., Ltd. (China). Deionized water (DI water) was obtained through laboratory preparation.

1.2 Synthesis of Materials

In detail, $Ni(NO_3)_2·6H_2O$ (15 mmoL) and $Fe(NO_3)_3·9H_2O$ (5 mmoL) were added to 100 mL of deionized water without CO_2 and constantly stirred at room temperature. Urea (50 mmoL) and NH_4F (25 mmoL) were slowly added to the above mixture, and stirring was continued for 60 minutes. The mixture was transferred to a 100 mL autoclave and placed in an oven at 120°C for 12 hours. The reacted solid is washed several times by centrifugation until the pH = 7.0 of the washing solution. The washed solids were dried at 60°C for 24 hours. The dried material was ground, sieved (200 mesh sieve), collected, and named NiFe-LDH.

Compared with NiFe-LDH, the synthesis process of modified NiFe-LDH has some differences. Firstly, glutamic was added to 50 mL of deionized water without CO_2. Control the pH range at 9.5 ~ 10.5 by adding 2.0 mol/L of NaOH dropwise to the mixed solutions (the mixed solution is named: A). $Ni(NO_3)_2·6H_2O$ (15.0 mmoL) and $Fe(NO_3)_3·9H_2O$ (5.0 mmoL) were added to 100 mL of deionized water without CO_2 and constantly stirred at room temperature (the mixed solution is named: B). Secondly, solution B was added slowly dropwise to A with constant stirring at 20°C. The pH range of the mixed solution was maintained at 9.5 ~ 10.5 by adding 2.0 mol/L NaOH dropwise to the

solution. The mixture was stirred for 30 minutes at 20°C, then transferred to a 100 mL reaction vessel and held at 120°C for 12 hours. Finally, in the same manner as NiFe-LDH, the solid product obtained was collected and named Glu@NiFe-LDH. The different glutamic-doped (glutamic: 2.5 mmoL, 5 mmoL, and 10 mmoL) composites were prepared by the same method.

1.3 Material characterization and instrumentation

The crystal structure of all materials was characterized by X-ray diffraction (Bruker D8 advance, Germany) with Cu Kα radiation (λ=1.5406 Å) at a scan rate of 0.05 °/s. The surface functional groups of the material were analyzed by Fourier transform infrared spectroscopy (FT-IR) (Nicolet IS-10, Thermo Fisher Scientific, USA) in the range 4000-500 cm^{-1}. The weight loss ratio of the material at different temperatures was analyzed by means of a thermogravimetric (TG) (TGA5500). The sample was heated at a rate of 10 °C/min under N_2. The chemical energy levels of surface elements of the materials were determined by X-ray photoelectron spectroscopy (XPS, ESCALAB250Xi, Thermo Fisher). The specific surface area and pore diameter of the material was analyzed by Brunauer-Emmett-Teller (BET). The Zeta potential of samples was performed on Zeta sizer Nano ZS90 (Malvern Instruments, UK).

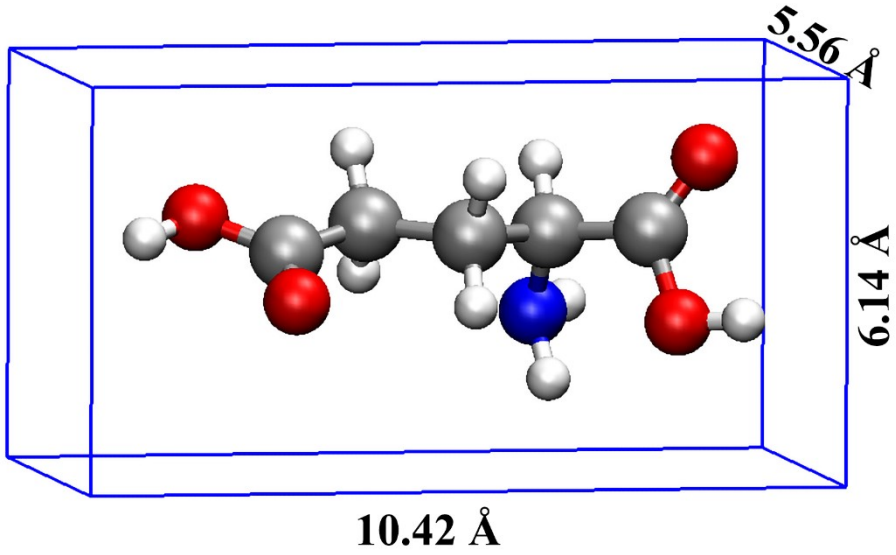

Figure S1. Molecular kinetic diameter of glutamic.

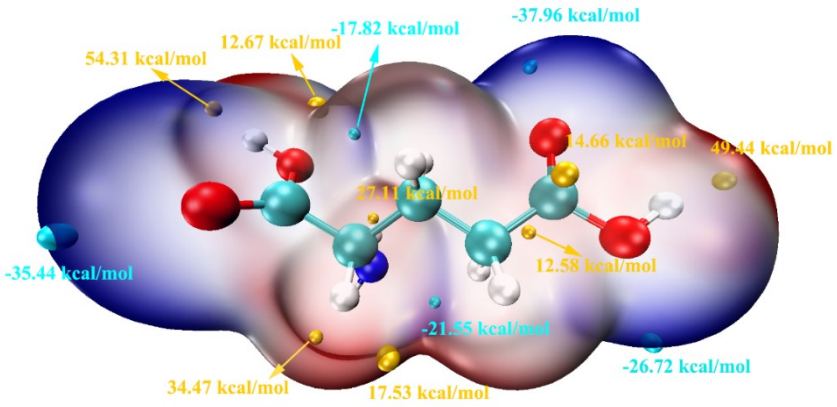

Figure S2. ESP mapped molecular vdW surface of glutamic.

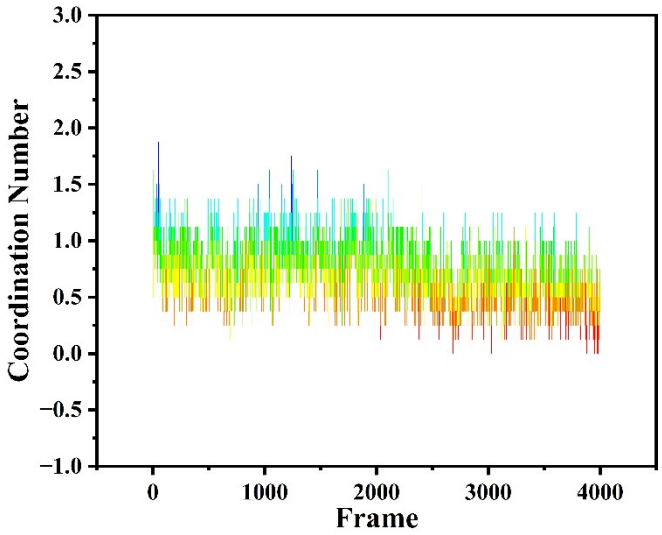

Figure S3. The variation of coordination number with the number of frames.

Table S1 . Parameters of Langmuir and Freundlich isotherm models for chromate adsorption by NiFe-LDH and Glu@NiFe-LDH.

T / *Model*		Langmuir			Freundlich		
		K_L	R^2	q_m	K_F	n	R^2
NiFe-LDH	**25°C**	0.1154	0.9798	43.42	16.57	5.5641	0.7141
	35°C	0.1434	0.9813	48.02	19.89	6.0023	0.6996
	45°C	0.2547	0.9395	51.93	24.46	6.6402	0.8256
Glu@NiFe-LDH	**25°C**	0.1247	0.9596	94.39	32.32	4.8497	0.8634
	35°C	0.2124	0.9671	113.82	42.33	4.9658	0.8939
	45°C	0.2384	0.9250	135.51	53.82	5.2569	0.9269