Supporting information

A review on fabricating heterostructures by layered double hydroxides for enhanced photocatalytic activities

M.J. Wu,[a,#] J.Z. Wu,[a,#] J. Zhang,[*,a,b] H. Chen,[a] J.Z. Zhou,[a] G.R. Qian,[**,a] Z. P. Xu,[c] Z. Du,[d] and Q.L. Rao [d]

[a] SHU Center of Green Urban Mining & Industry Ecology, School of Environmental and Chemical Engineering, Shanghai University, No. 333 Nanchen Rd., Shanghai 200444, P. R. China;

[b] Shanghai Institute of Materials Genome, Shanghai, No. 99 Shangda Rd., Shanghai 200444, P. R. China;

[c] ARC Centre of Excellence for Functional Nanomaterials, Australian Institute for Bioengineering and Nanotechnology, the University of Queensland, Brisbane, QLD 4072, Australia;

[d] National Supercomputing Center in Shenzhen, Guangdong, Shenzhen 51800, P. R. China.

[#] These authors contributed equally.

Table S1. Lattice parameters of calculated LDHs

	a	b	c	D=c/3
$Mg_{2.0}Al\text{-}Cl^-$	18.399	6.131	22.673	7.558
$Mg_{2.6}Al\text{-}Cl^-$	18.410	6.172	22.628	7.543
$Mg_{3.5}Al\text{-}Cl^-$	18.427	6.181	22.766	7.589
$Mg_{2.0}Al\text{-}NO_3^-$	18.297	6.143	25.314	8.438
$Zn_{2.0}Al\text{-}Cl^-$	18.674	6.268	22.578	7.526
$Mg_{24}Al_9Ti_3\text{-}Cl^-$	18.535	6.178	22.503	7.501
$Mg_{24}Al_{11}Ti\text{-}Cl^-$	18.468	6.153	22.708	7.569
$Mg_{2.0}Cr\text{-}Cl^-$	18.439	6.253	22.800	7.600

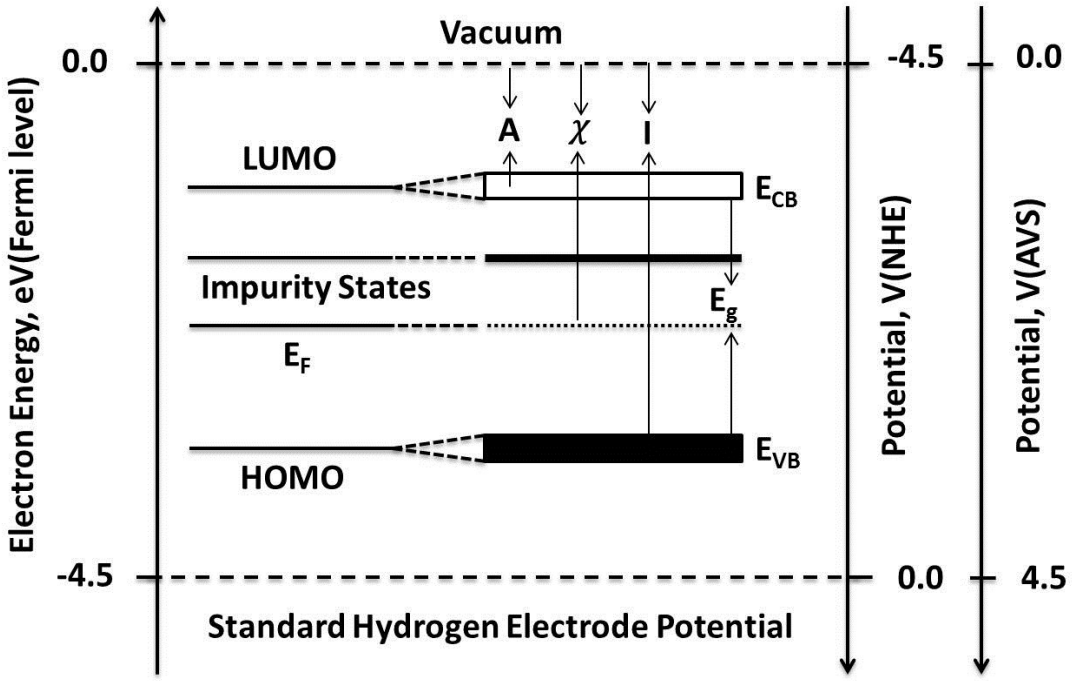

Figure S1. Conversion relation between absolute vacuum energy scale (V/AVS) and normal hydrogen electrode (V/NHE).
Fermi level (eV) is electrochemical potential of electron on electrode; E_{CB} is conduction band edge; E_{VB} is valence band edge; E_g is band gap; E_F is Fermi level; LUMO is lowest unoccupied molecular orbital; HOMO is highest occupied molecular orbital.[1-7]

The band gaps from KS-DFT+U were not directly related to any actual measurements. Such band gaps as “eigenvalue gaps”, which were the difference between LUMO and HOMO in KS (Kohn-Sham) eigenvalues. Energy zero was set to the Fermi energy during calculation of DOS. The positions of E_{VB} and E_{CB} with respect to the normal hydrogen electrode (NHE) were computed according to Eq.1-4.

$$E_{CB} = X - 0.5E_g + E_0 \qquad \text{Eq.1}$$

$$E_{VB} = X + 0.5E_g + E_0 \qquad \text{Eq.2}$$

$$X = (\chi_B^b \chi_C^c)^{1/(b+c)} \qquad \text{Eq.3}$$

$$\chi = \frac{E_I + E_A}{2} \qquad \text{Eq.4}$$

Where E_g was the band gap energy; E_0=-4.5 eV for normal hydrogen electrode; X was the electronegativity of solid material (such as B_bC_c compound), which was expressed as the geometric mean of absolute electronegativity of the constituent atoms. The absolute electronegativity of each atom was obtained from other literatures;[8,9] χ_B and χ_C were the absolute electronegativity of atoms B and C. E_I and E_A were the ionization energy and electric affinity of atom.

Besides, electrostatic potential of Zn_2Al-LDH (001) surface was calculated by DFT+U. There was a 15 Å of vacuum region on the surface, where the electrostatic potential energy was set to zero to set the vacuum level. The position of valence-band as $E_{VB(vacuum)}$ can be obtained using the Fermi level and the vacuum level. The difference of E_{VB} and $E_{VB(vacuum)}$ was around 0.3 eV. Therefore, above calculations were convincing.

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