Electronic Supplementary Material (ESI) for Dalton Transactions.


# Adsorption-photoreduction behaviors and mechanisms of layered double hydroxide loaded on uranium(VI) removal

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## 1. The calculation formula

The adsorption data were simulated by the pseudo-first-order and the pseudo second-order models and Langmuir and Freundlich models by Eq. (1-5), respectively.

$$\ln(q_e - q_t) = \ln q_e - k_1 t \quad (1)$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \quad (2)$$

$$q_t = k_p t^{1/2} + C \quad (3)$$

$$q_e = \frac{K_L q_{max} C_e}{K_L C_e + 1} \quad (4)$$

$$q_e = K_F C_e^{1/n} \quad (5)$$

Where, $q_t$ (mg/g) and $q_{max}$ (mg/g) were the amount of U(VI) at contact time and the theoretical maximum adsorption capacity, respectively. $k_1$ ($min^{-1}$) and $k_2$ (g/mg·min) were separately the rate constants of kinetic models, as well as $K_L$ (L/mg) and $K_F$ ($mg^{1-1/n}·g^{-1}·L^{-1/n}$) were the equilibrium constants of Langmuir and Freundlich models, respectively.

The change of Gibbs free energy ($\Delta G^0$), entropy ($\Delta S^0$) and enthalpy ($\Delta H^0$) were calculated by Eq. (6-8).

$$\Delta G^0 = -RT \ln K_0 \quad (6)$$

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \quad (7)$$

$$\ln K_0 = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT} \quad (8)$$

Where, $K_0$ was the thermodynamic equilibrium constant; $R$ was the ideal gas constant 8.314 J/(mol·K) and $T$ was absolute temperature (K).

## 2. Figures

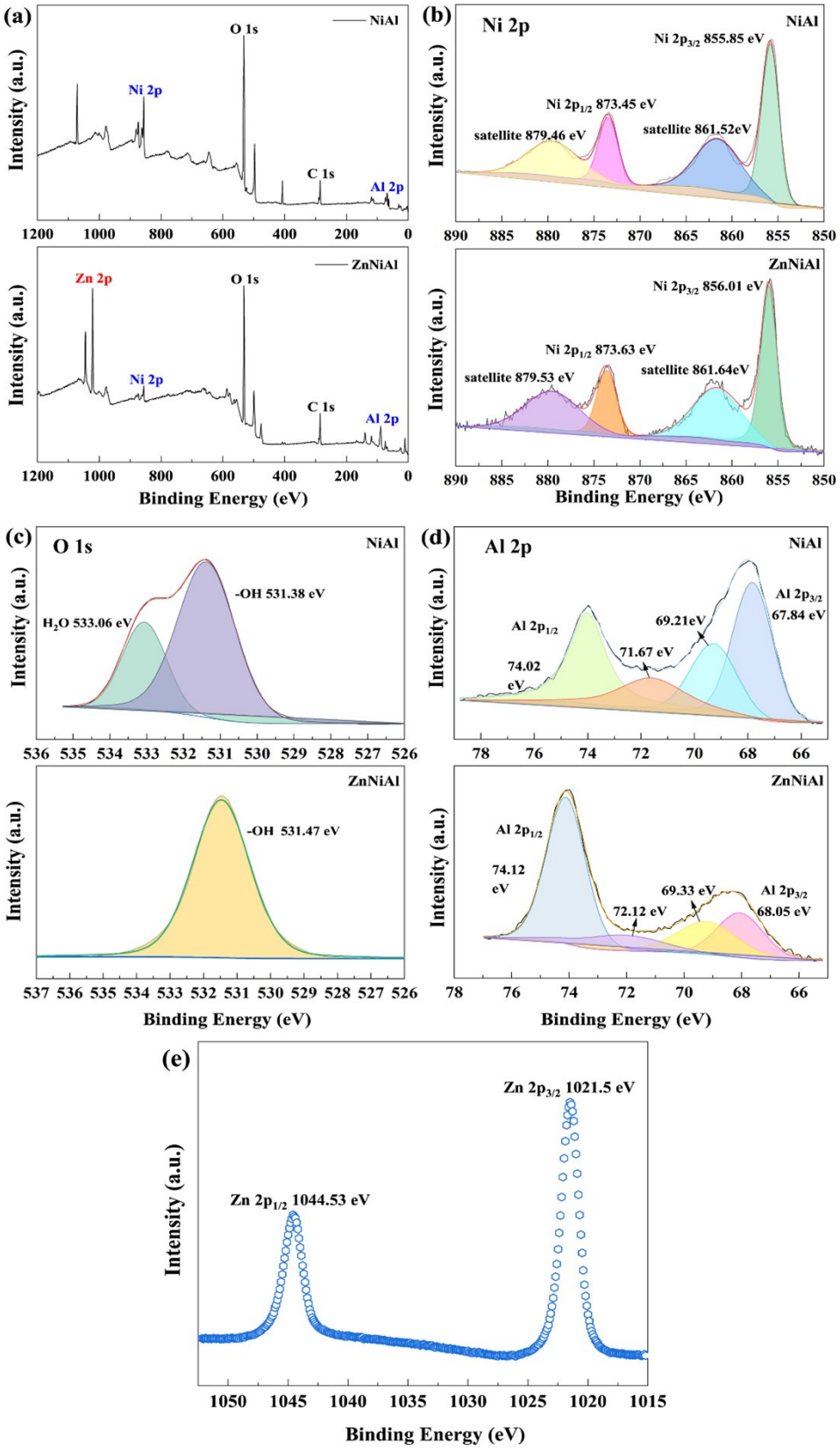


Fig. S1 The high-resolution XPS spectra of NiAl and ZnNiAl: (a) survey (b) Ni 2p, (c) O 1s, (d) Al 2p and (e) Zn 2p.

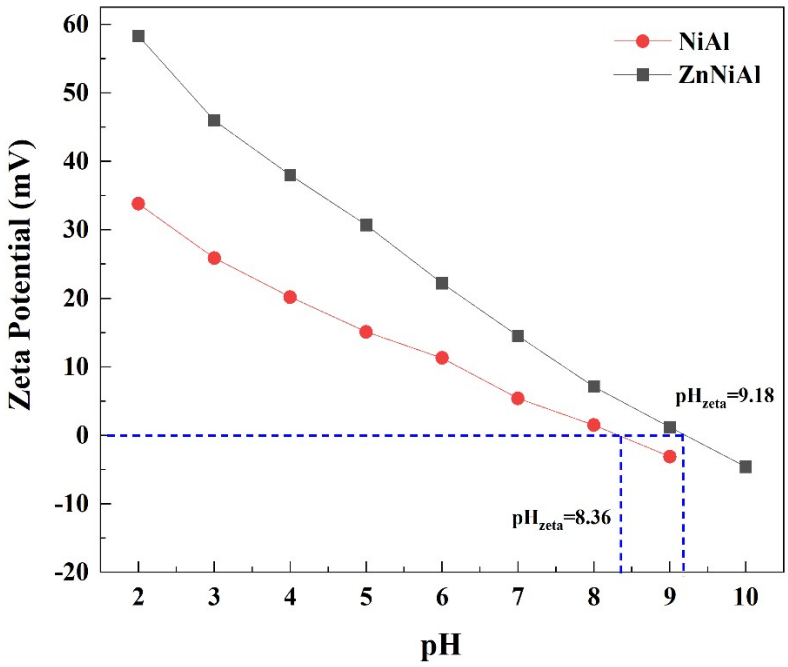


Fig. S2 The positive zeta potential value of NiAl and ZnNiAl.

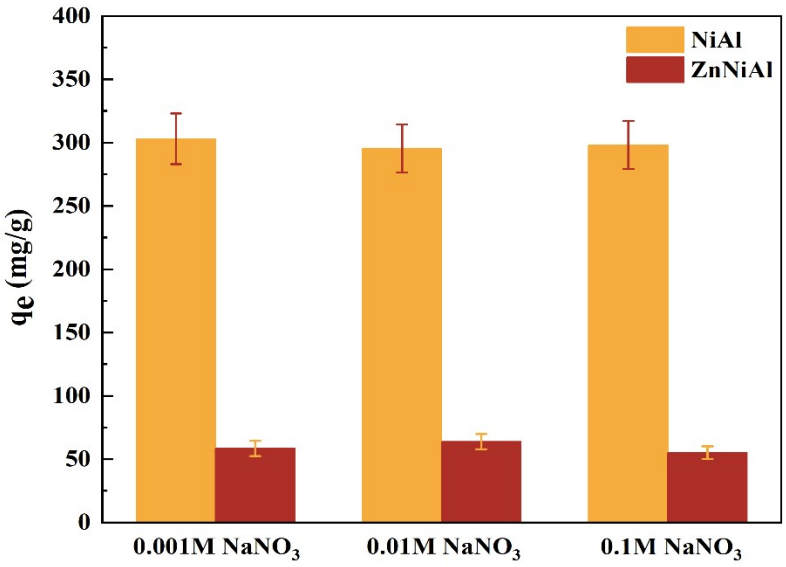


Fig. S3 The different concentrations of $NaNO_3$ on U(VI) adsorption over NiAl and ZnNiAl.

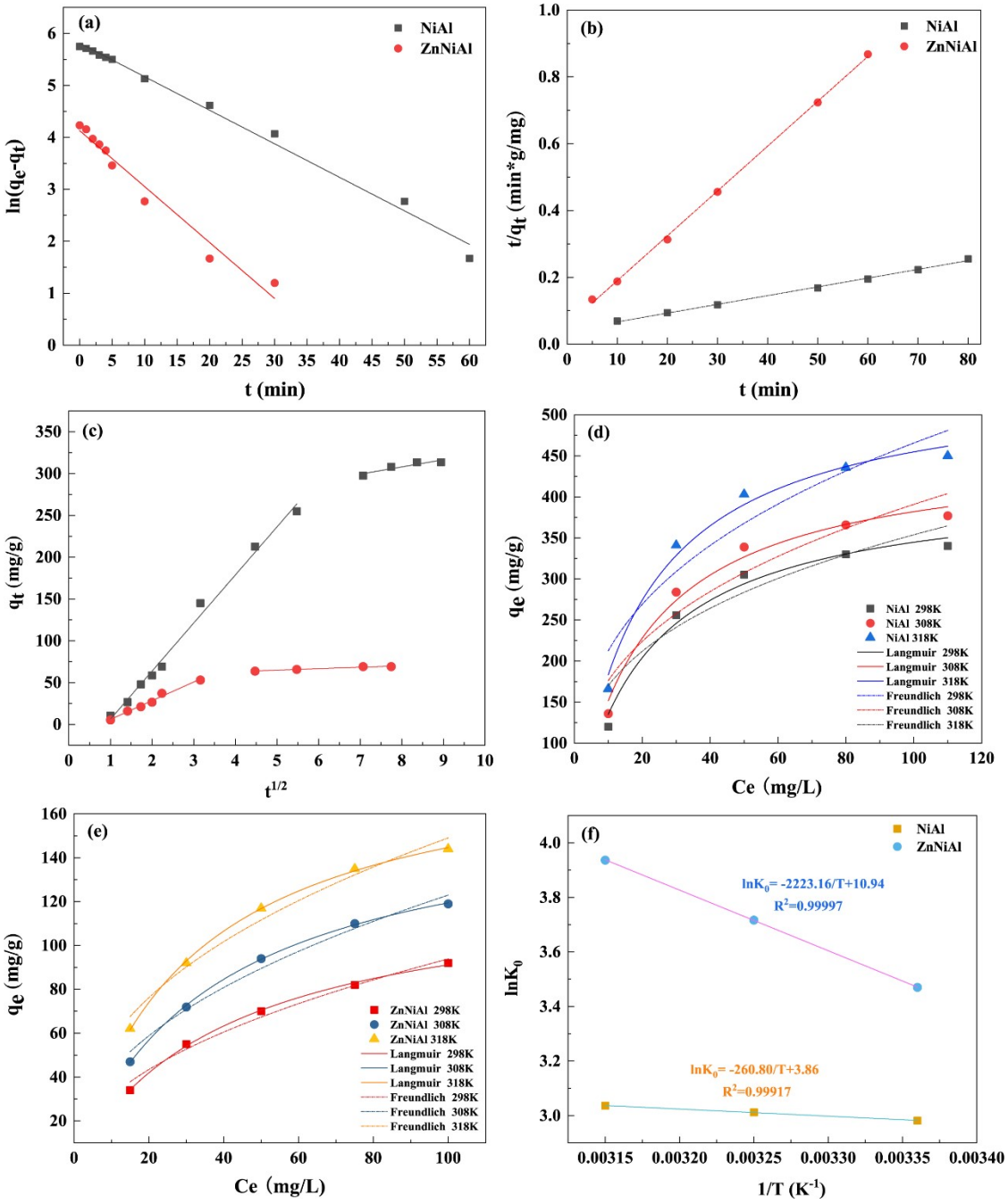


Fig. S4 The adsorption kinetics of U(VI) ($C_0$=50 mg/L, T=298-318 K, pH=6.0, m=2 mg, V=100 mL) (a) the pseudo-first-order model; (b) the pseudo-second-order model; (c) the intra-particle diffusion model; (d) the Langmuir model; (e) the Freundlich model; (f) the linear plot of $\ln K_0$ versus 1/T at three different temperatures.

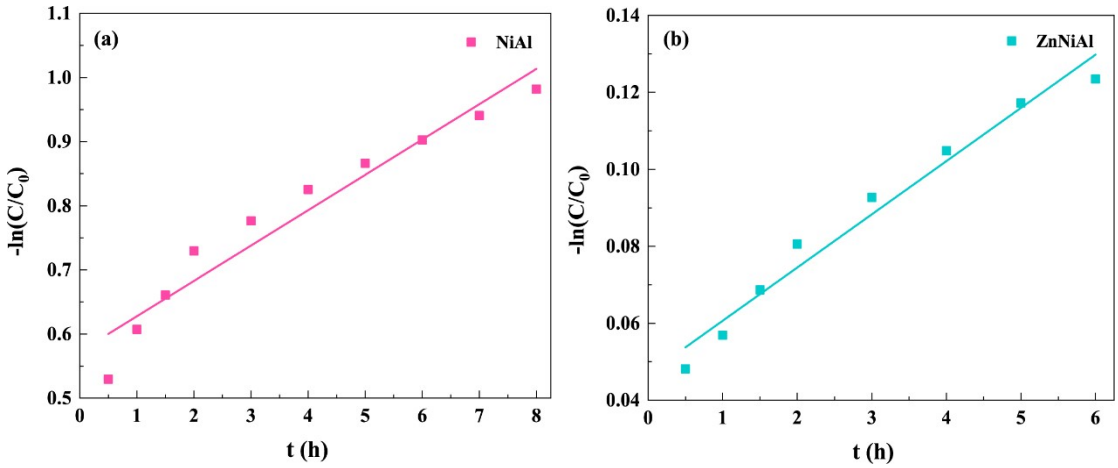

Fig. S5 The rate constants (k) of U(VI) photoreduction on NiAl and ZnNiAl.

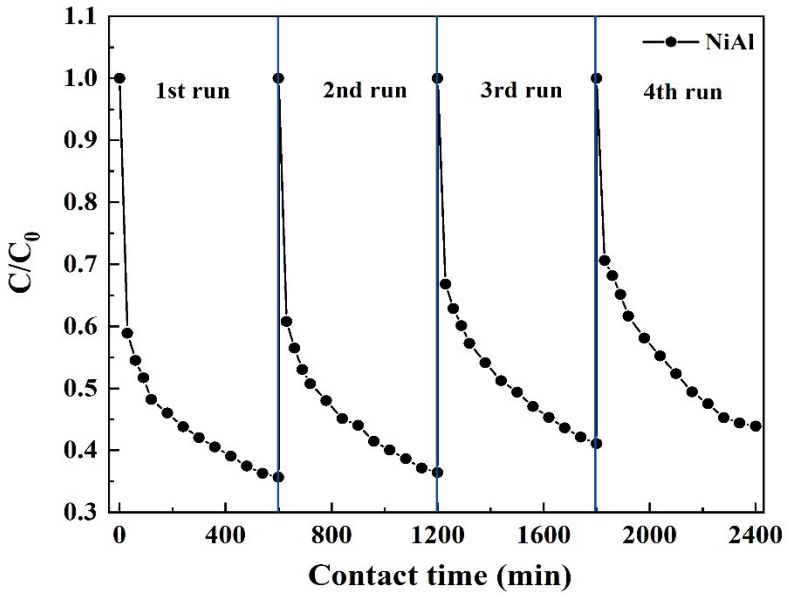


Fig. S6 The recyclability tests of visible-light driven photocatalytic activity for U(VI) over NiAl.

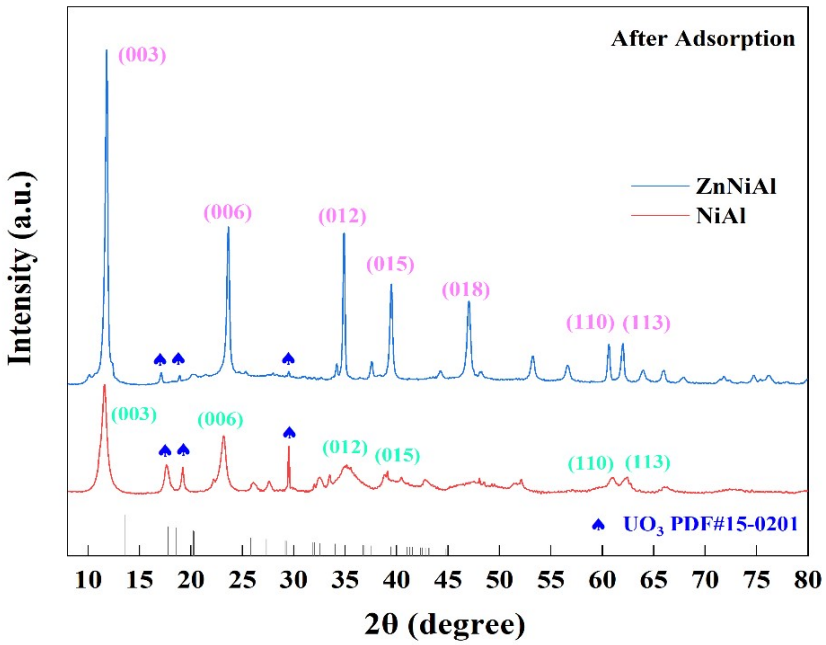


Fig. S7 The XRD spectra of NiAl and ZnNiAl after adsorption.

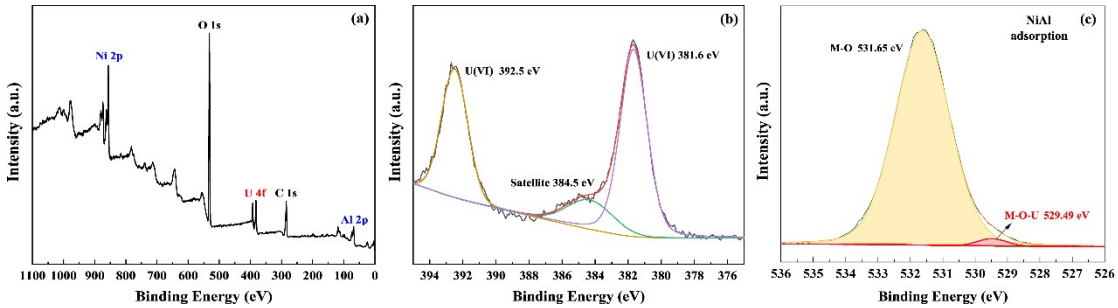


Fig. S8 The XPS survey, U4f and O1s spectra of NiAl-LDHs after adsorption.