Supporting Information

Mono-Transition-Metal-Substituted Polyoxometalate Intercalated Layered Double Hydroxides for the Catalytic Decontamination of Sulfur Mustard Simulant

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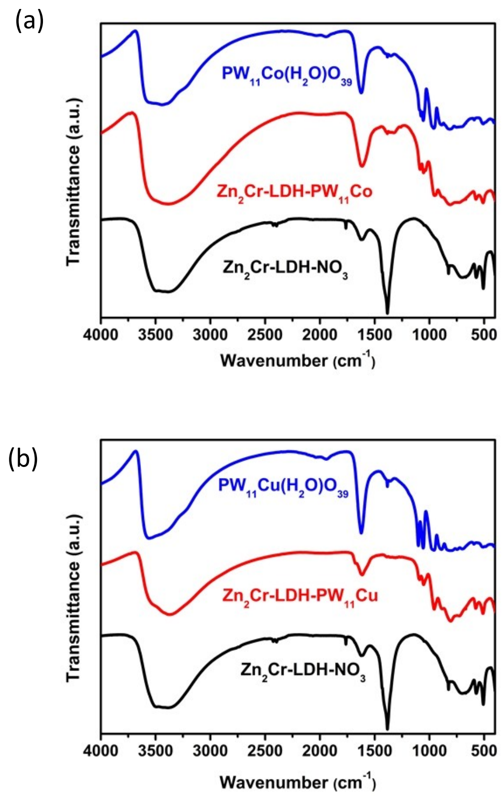


Figure S1. (a) FT-IR spectra of Zn_2Cr-LDH-$PW_{11}Co$; (b) FT-IR spectra of Zn_2Cr-LDH-$PW_{11}Cu$.

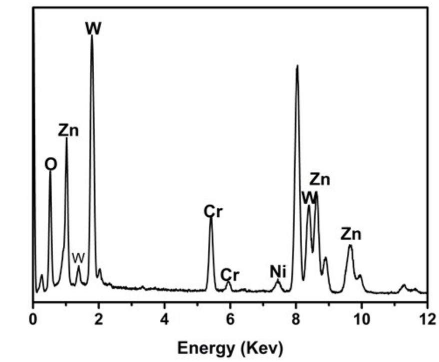


Figure S2. EDS of Zn_2Cr-LDH-$PW_{11}Ni$.

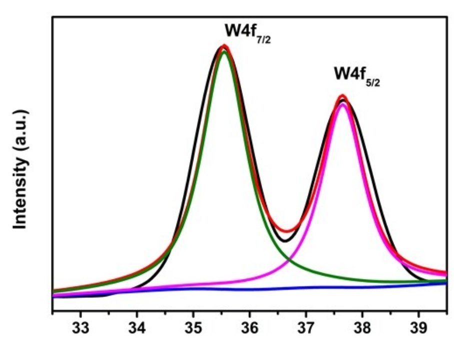
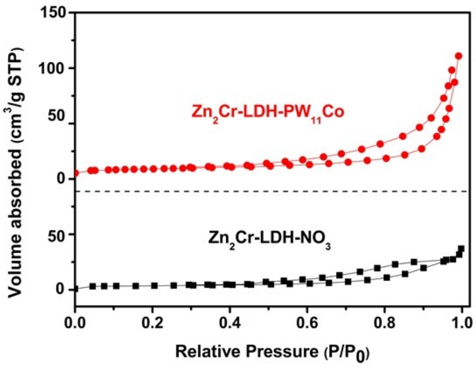


Figure S3. XPS spectra for the W4f core level spectrum of Zn_2Cr-LDH-$PW_{11}Ni$.

(a)



(b)

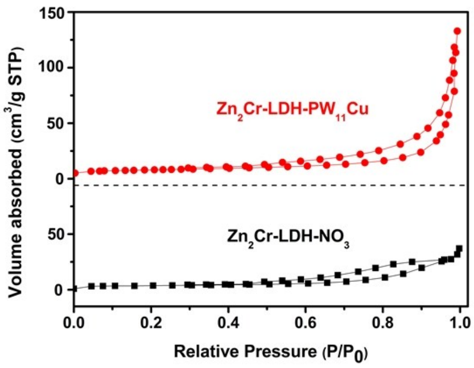


Figure S4. (a) N_2 adsorption-desorption isotherms of Zn_2Cr-LDH-$PW_{11}Co$; (b) N_2 adsorption-desorption isotherms of Zn_2Cr-LDH-$PW_{11}Cu$.

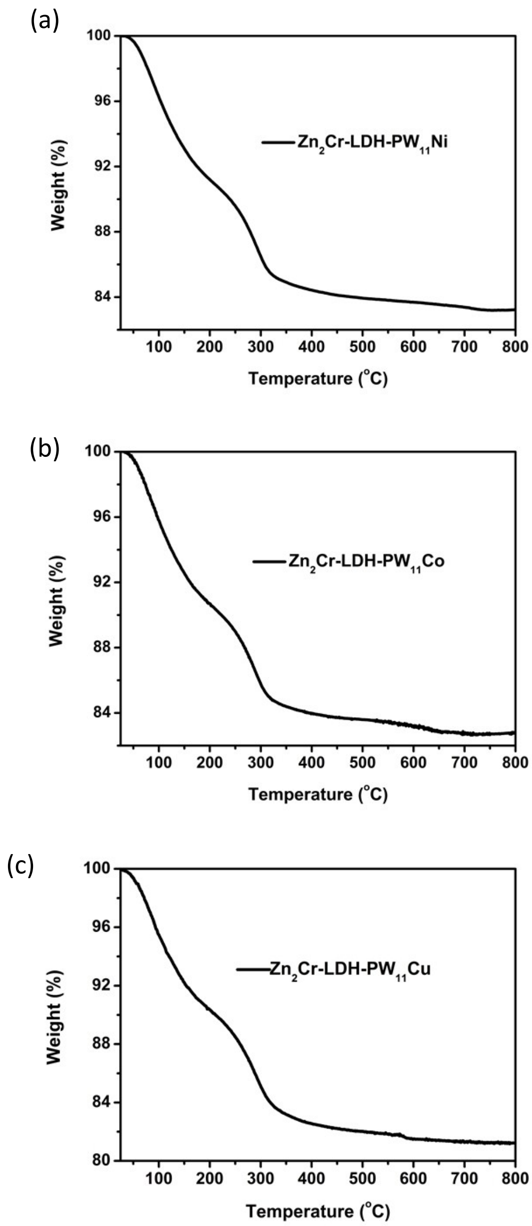


Figure S5. (a) TG analysis of Zn_2Cr-LDH-$PW_{11}Ni$; (b) TG analysis of Zn_2Cr-LDH-$PW_{11}Co$. (c) TG analysis of Zn_2Cr-LDH-$PW_{11}Cu$.

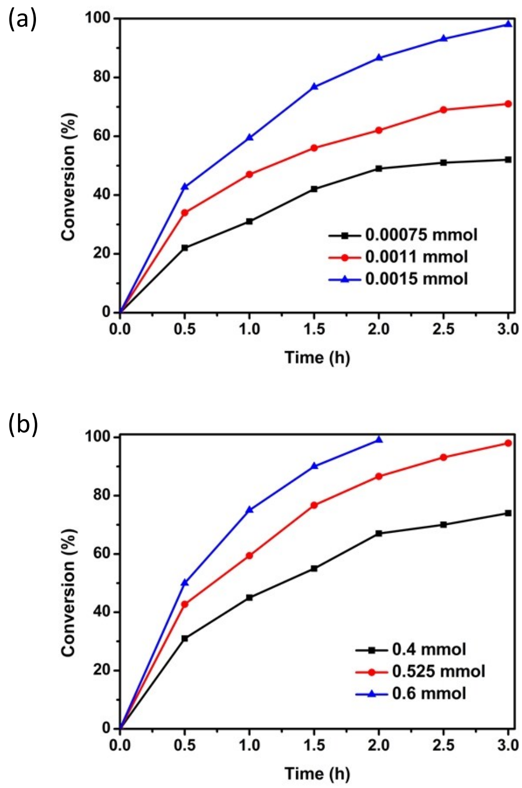


Figure S6. (a) Decontamination of CEES with different amounts of Zn_2Cr-LDH-$PW_{11}Ni$. Reaction conditions: Zn_2Cr-LDH-$PW_{11}Ni$, CEES (0.5 mmol), 1,3-dichlorobenzene (0.25 mmol), 3% aqueous H_2O_2 (0.525 mmol) and acetonitrile (4 mL) at room temperature; (b) Decontamination of CEES with different amounts of 3% aqueous H_2O_2. Reaction conditions: Zn_2Cr-LDH-$PW_{11}Ni$ (0.0015 mmol), CEES (0.5 mmol), 1,3-dichlorobenzene (0.25 mmol), 3% aqueous H_2O_2 and acetonitrile (4 mL) at room temperature.

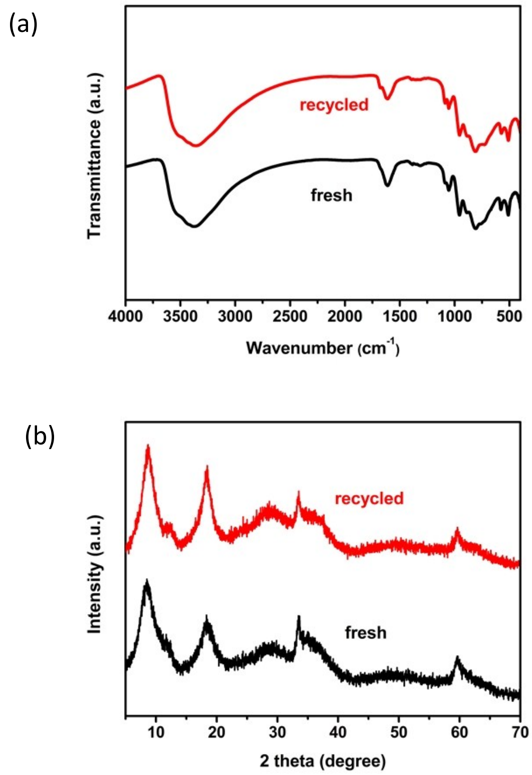


Figure S7. (a) FT-IR spectra of recycled Zn_2Cr-LDH-$PW_{11}Ni$ and fresh Zn_2Cr-LDH-$PW_{11}Ni$; (b) PXRD spectra of recycled Zn_2Cr-LDH-$PW_{11}Ni$ and fresh Zn_2Cr-LDH-$PW_{11}Ni$.

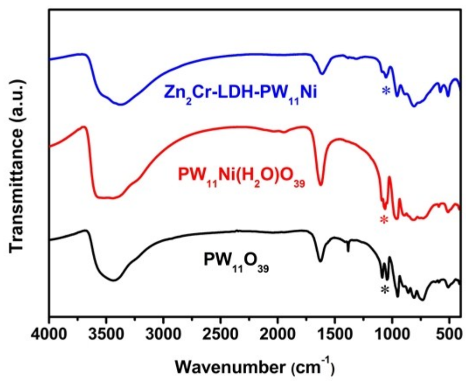


Figure S8. FT-IR spectra of Zn_2Cr-LDH-$PW_{11}Ni$, $PW_{11}Ni$ and $PW_{11}O_{39}$. The P-O band splitting of Zn_2Cr-LDH-$PW_{11}Ni$ (marked with blue star) was obviously weaker than that of $PW_{11}O_{39}$ (marked with black star), indicating that PW11Ni keeps integrity during intercalation process.[1, 2]

Table S1. The oxidation of CEES catalyzed by Zn_2Cr-LDH-$PW_{11}Ni$ with adding radical scavengers.

Radical scavengers	Time (h)	Conversion (%)
-	3	98
p-benzoquinone (•O2−/•O_2H)	3	94
tert-butyl alcohol (•OH)	3	98
diphenylamine (•OH)	3	98

Reaction conditions: CEES (0.5 mmol), 1,3-dichlorobenzene (internal standard, 0.25 mmol), radical scavengers (0.5 mmol) and Zn_2Cr-LDH-$PW_{11}Ni$ (0.0015 mmol) were dispersed in acetonitrile (4 mL). After mixing evenly, 3 % aqueous H_2O_2 (0.525 mmol) was added to initiate the reaction.

References

1 F. Zonnevijlle, C. M. Touren, and G. F. Touren, *Inorg Chem*, 1982, **21**, 2742–2750.

2 J. H. Choi, J. K. Kim, D. R. Park, T. H. Kang, J. H. Song and I. K. Song, *J Mol Catal A: Chem*, 2013, **371**, 111-117.