

Electronic Supplementary Information (ESI)

Multifunctional NaEu(WO₄)₂: defect-tuned red emission and acetone sensing at room temperature

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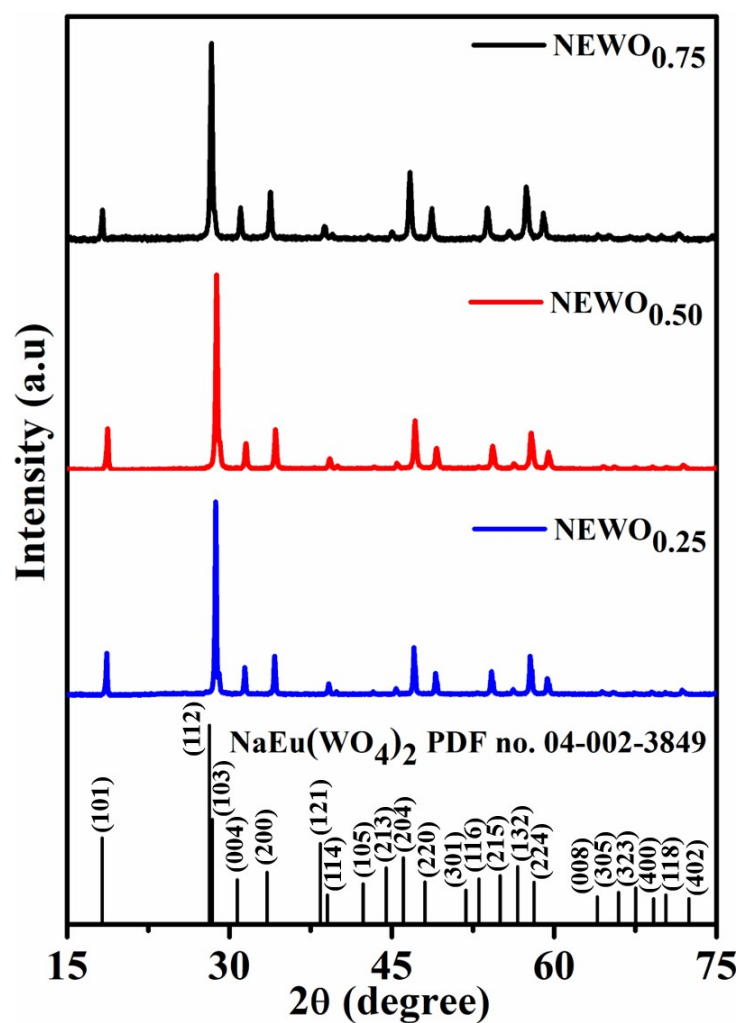


Figure S1 XRD spectrum of $\text{NEWO}_{0.75}$, $\text{NEWO}_{0.50}$ and $\text{NEWO}_{0.25}$ samples.

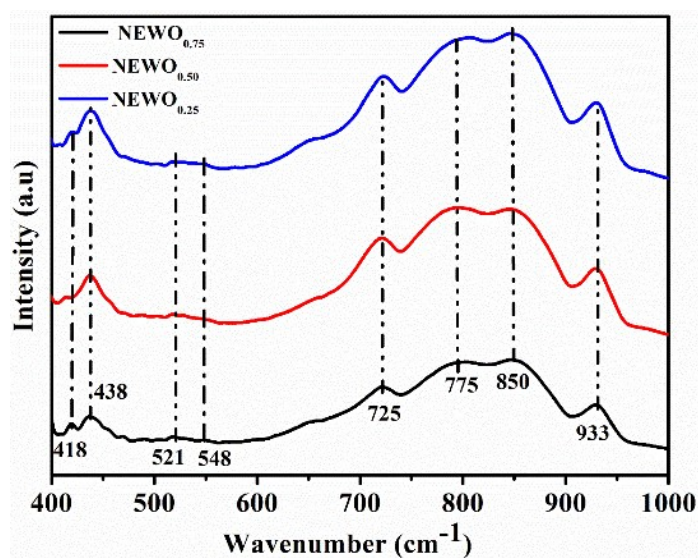


Figure S2 FTIR spectra of $\text{NEWO}_{0.75}$, $\text{NEWO}_{0.50}$ and $\text{NEWO}_{0.25}$ samples.

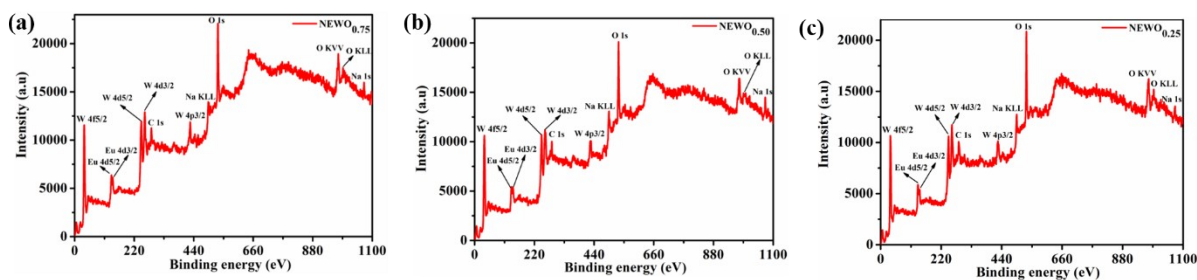


Figure S3 XPS survey spectrum of (a) $\text{NEWO}_{0.75}$, (b) $\text{NEWO}_{0.50}$ and (c) $\text{NEWO}_{0.25}$ samples.

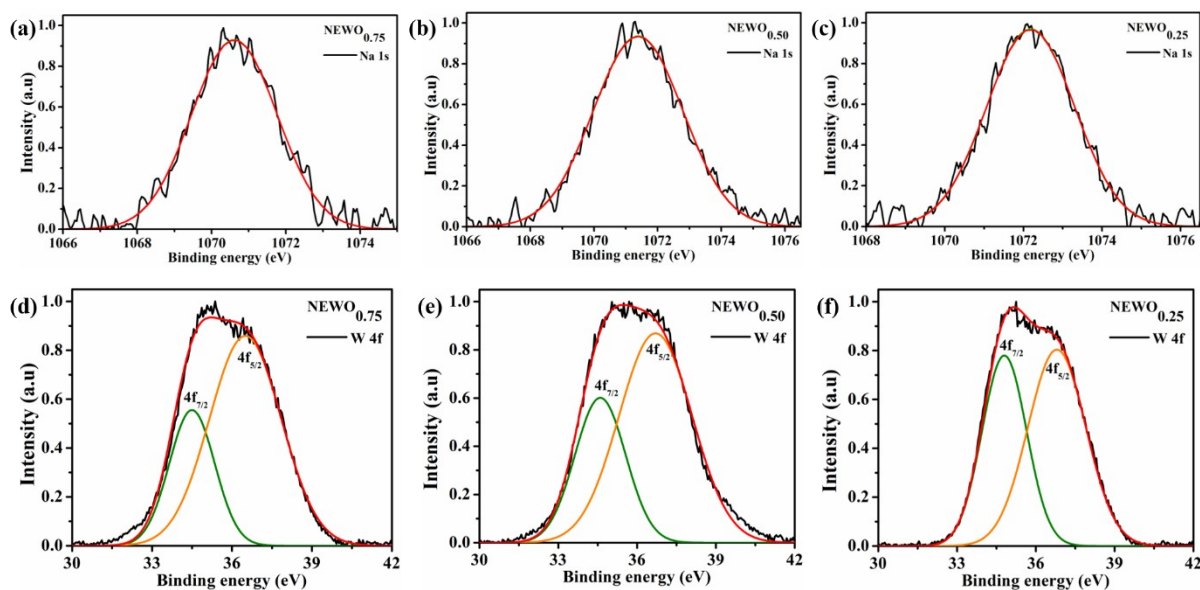


Figure S4 XPS high resolution spectra of Na 1s: (a) $\text{NEWO}_{0.75}$, (b) $\text{NEWO}_{0.50}$, (c) $\text{NEWO}_{0.25}$ samples and W 4f: (d) $\text{NEWO}_{0.75}$, (e) $\text{NEWO}_{0.50}$, (f) $\text{NEWO}_{0.25}$ samples.

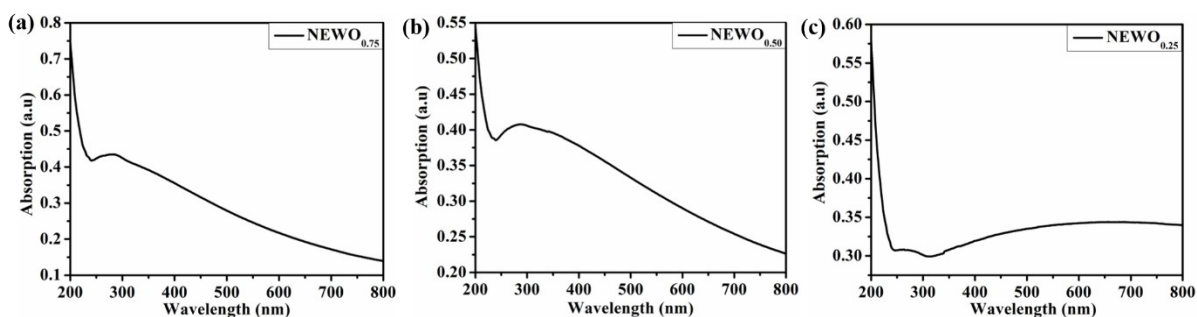


Figure S5 UV-Vis absorption spectra: (a) $\text{NEWO}_{0.75}$, (b) $\text{NEWO}_{0.50}$ and (c) $\text{NEWO}_{0.25}$ samples.

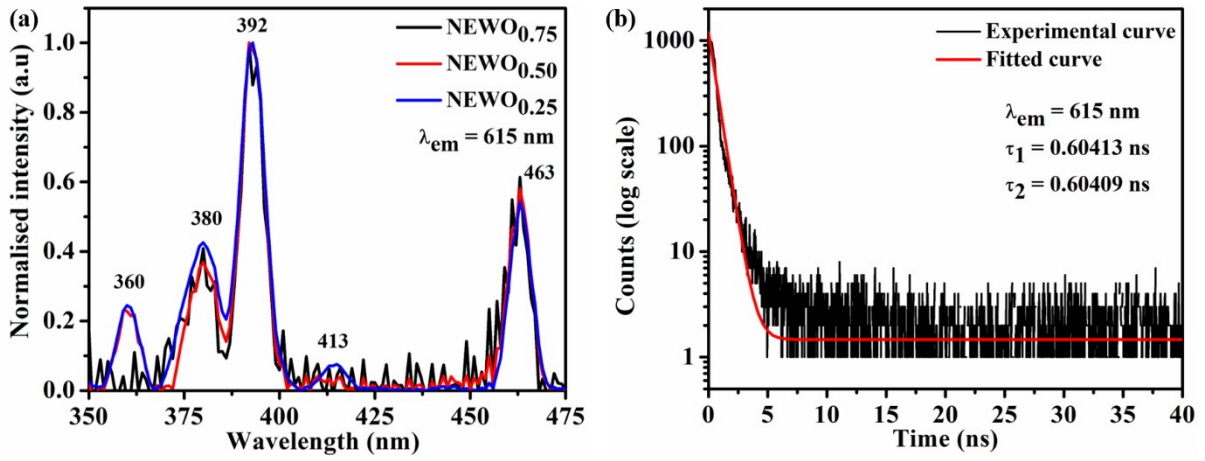


Figure S6 (a) PLE spectra of $\text{NEWO}_{0.75}$, $\text{NEWO}_{0.50}$ and $\text{NEWO}_{0.25}$ samples, (b) Decay curve of $\text{NEWO}_{0.25}$.

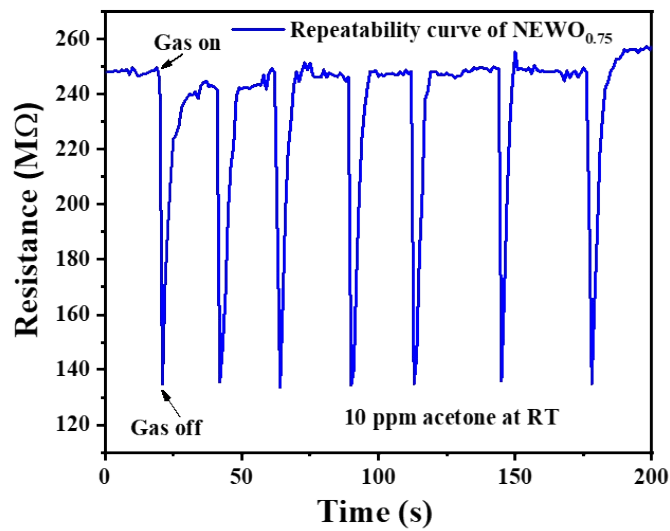


Figure S7 Repeatability data for $\text{NEWO}_{0.75}$ upon seven cycles of exposure to 10 ppm acetone at RT.

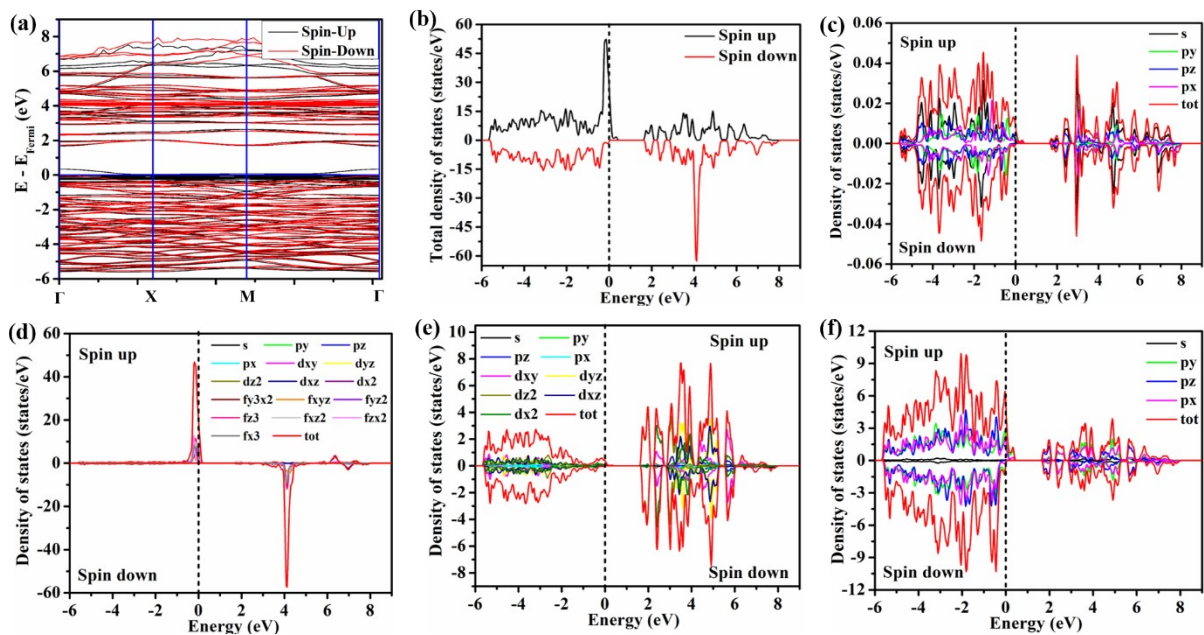


Figure S8 DFT of $\text{NEWO}_{0.25}$: (a) Band structure, (b) TDOS, (c) DOS of Na, (d) DOS of Eu, (e) DOS of W, (f) DOS of O.

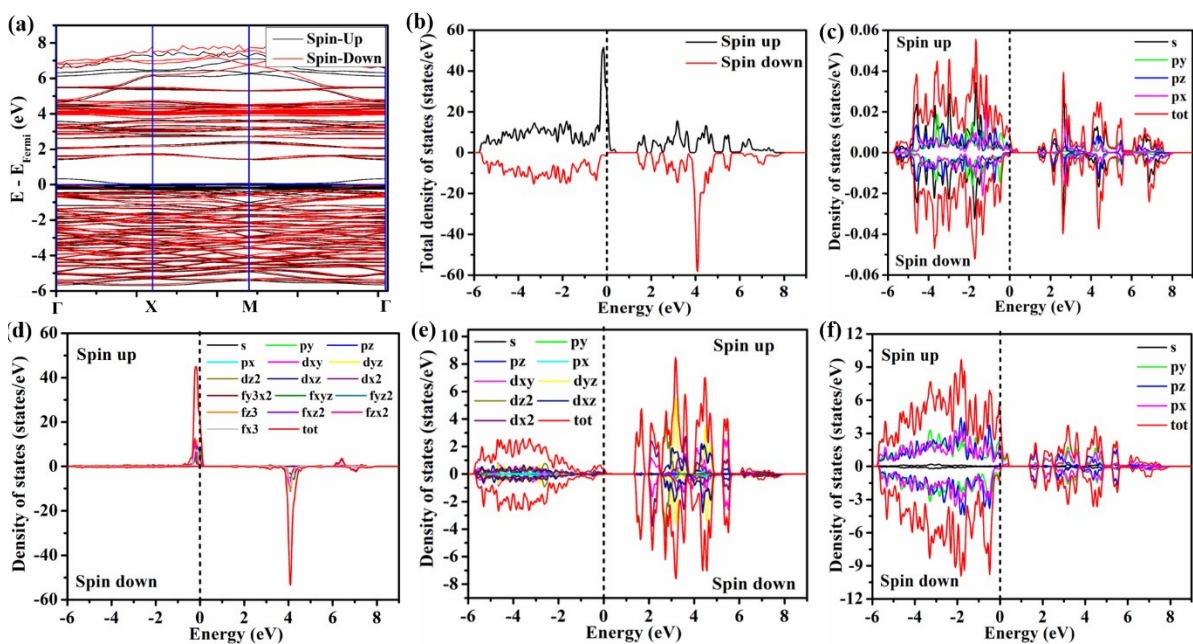


Figure S9 DFT of $\text{NEWO}_{0.50}$: (a) Band structure, (b) TDOS, (c) DOS of Na, (d) DOS of Eu, (e) DOS of W, (f) DOS of O.

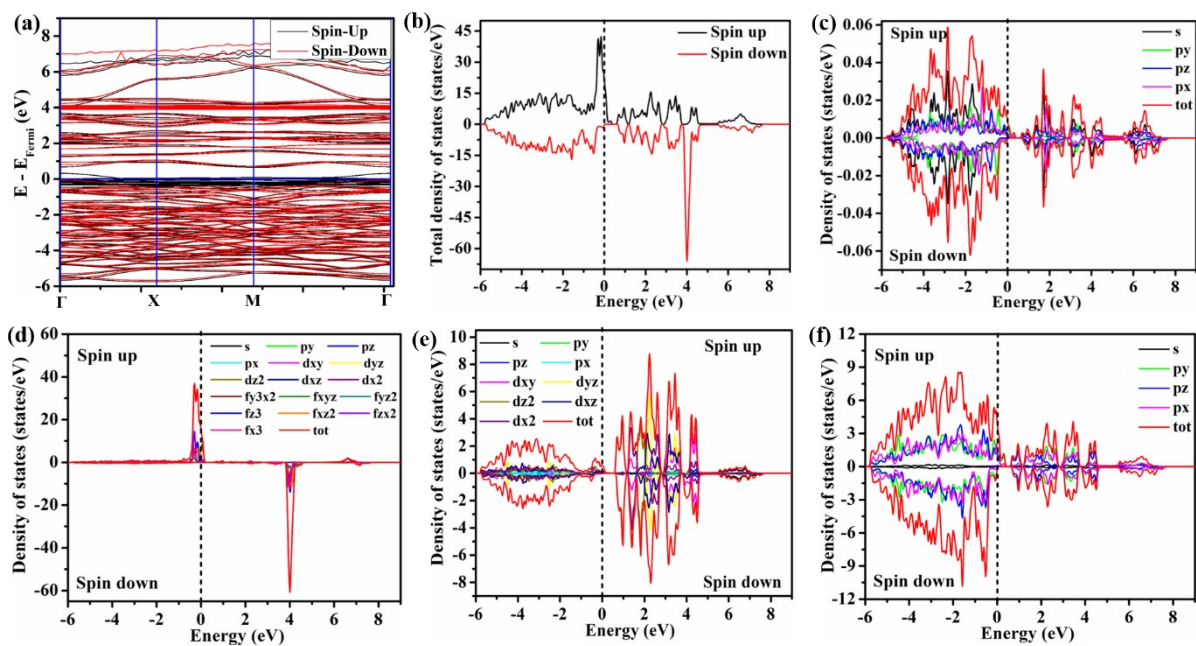


Figure S10 DFT of $\text{NEWO}_{0.75}$: (a) Band structure, (b) TDOS, (c) DOS of Na, (d) DOS of Eu, (e) DOS of W, (f) DOS of O.

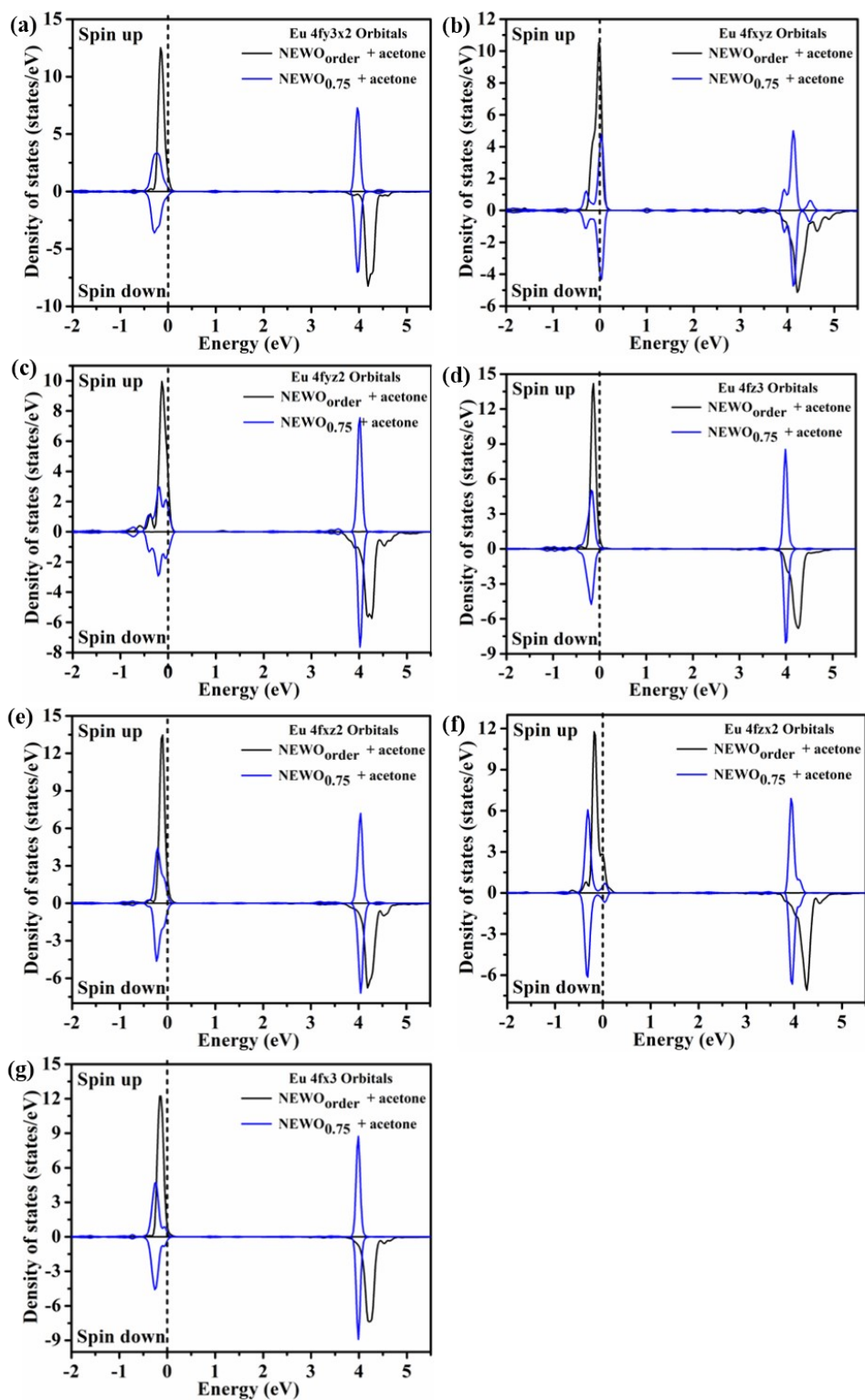


Figure S11 PDOS plot of (0 0 4) slab surface + acetone molecule: (a) Eu $4f_y^3x^2$ orbitals, (b) Eu $4f_{xyz}$ orbitals, (c) Eu $4f_{yz^2}$ orbitals, (d) Eu $4f_z^3$ orbitals, (e) Eu $4f_{xz^2}$ orbitals, (f) Eu $4f_{zx^2}$ orbitals, (g) Eu $4f_x^3$ orbitals.

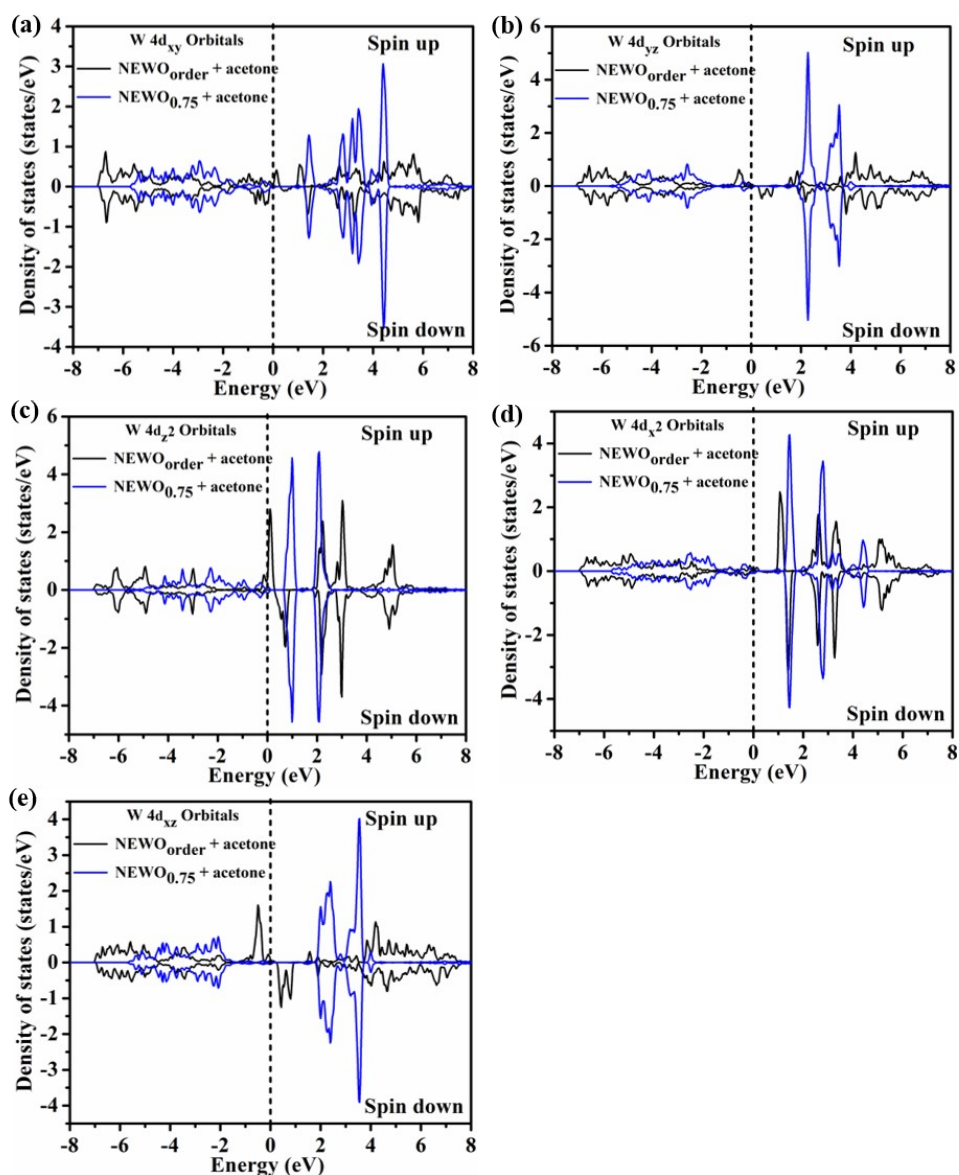


Figure S12 PDOS plot of (0 0 4) slab surface + acetone molecule: (a) W $4d_{xy}$ orbitals, (b) W $4d_{yz}$ orbitals, (c) W $4d_z^2$ orbitals, (d) W $4d_x^2$ orbitals, (e) W $4d_{xz}$ orbitals.