Supporting Information

Host–Guest Adsorption Energetics in Functionalized UiO-66 Nanocrystals for Selective VOCs Sensing

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S1- Supporting Figures

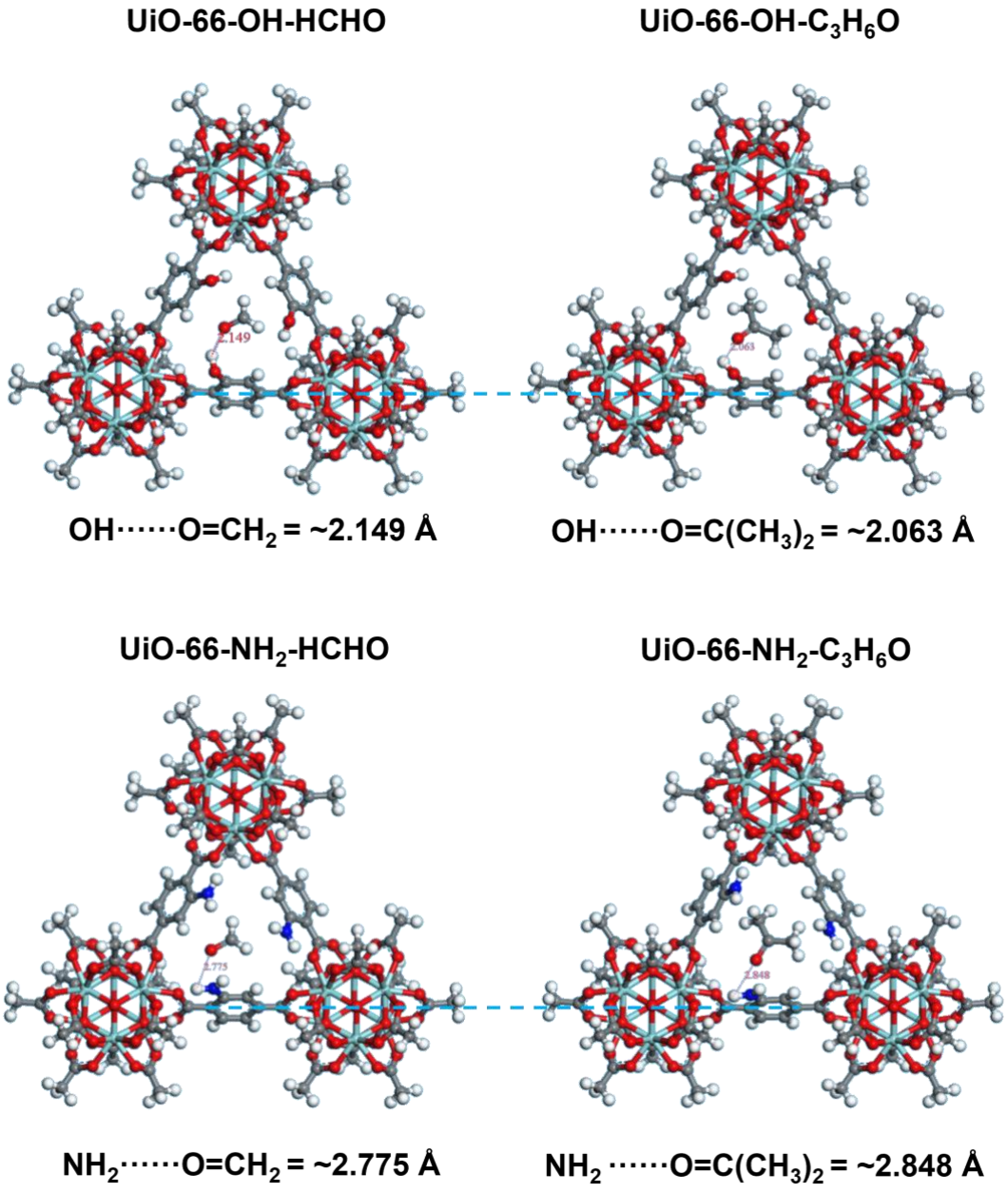

Figure S1. Optimized host–guest structures of HCHO and acetone C_3H_6O during translocation through the triangular windows of UiO-66-OH and UiO-66-NH_2.

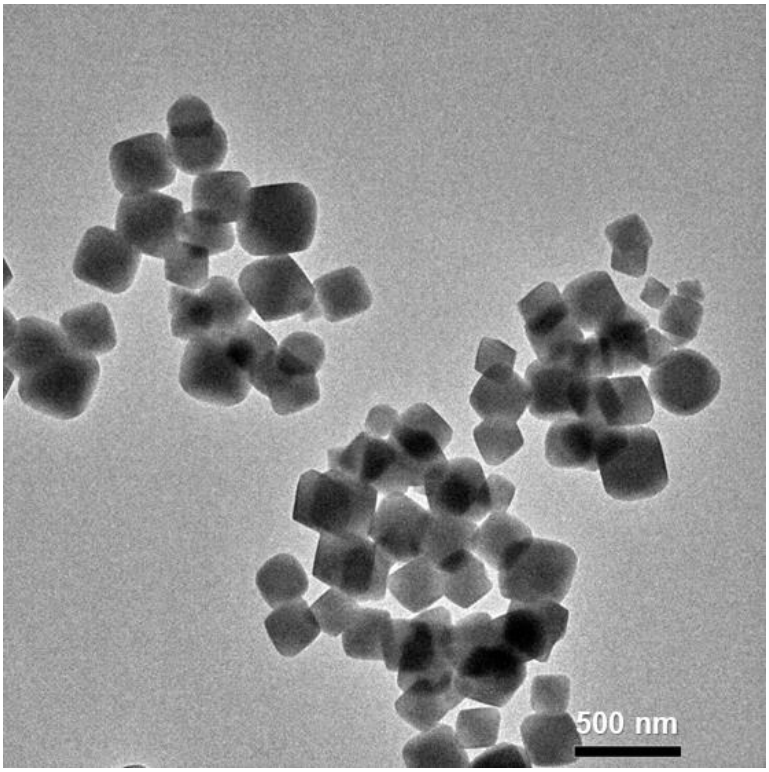

Figure S2. TEM image of UiO-66.

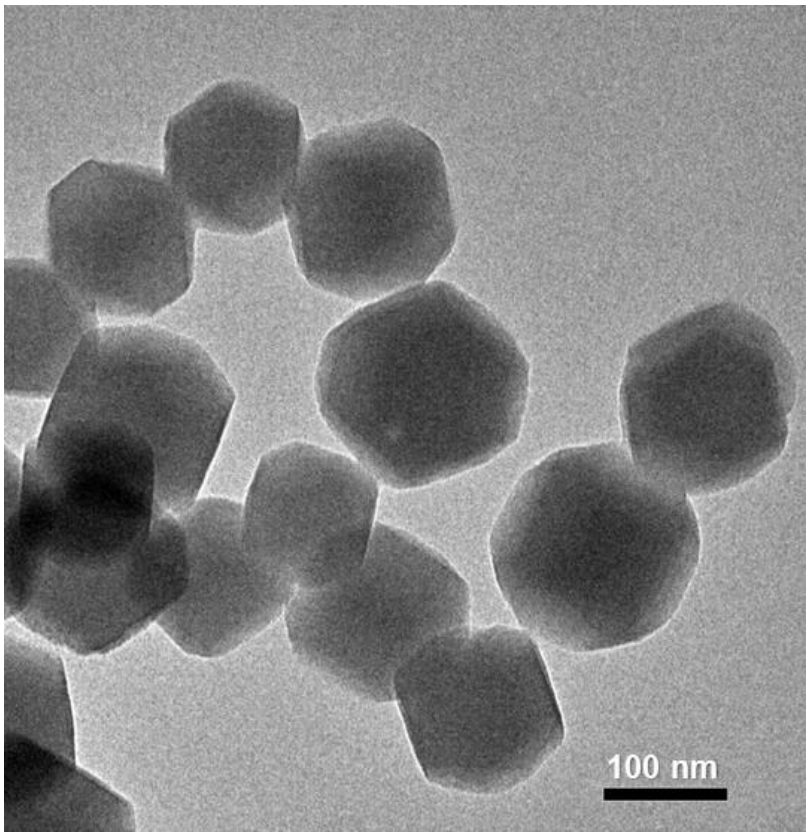

Figure S3. TEM image of UiO-66-NH_2.

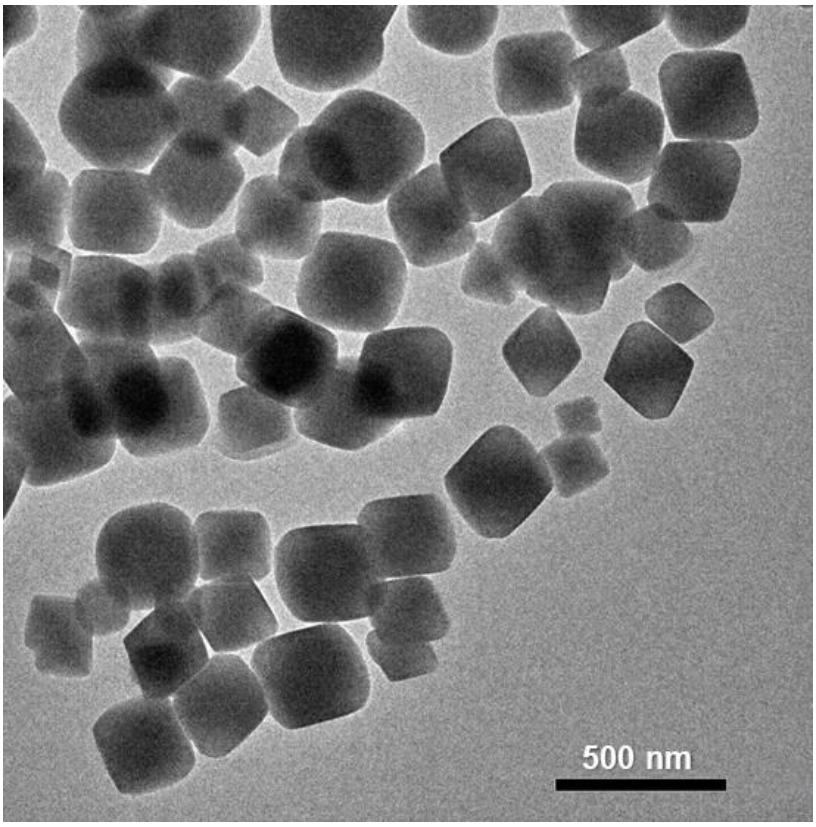

Figure S4. TEM image of UiO-66-OH.

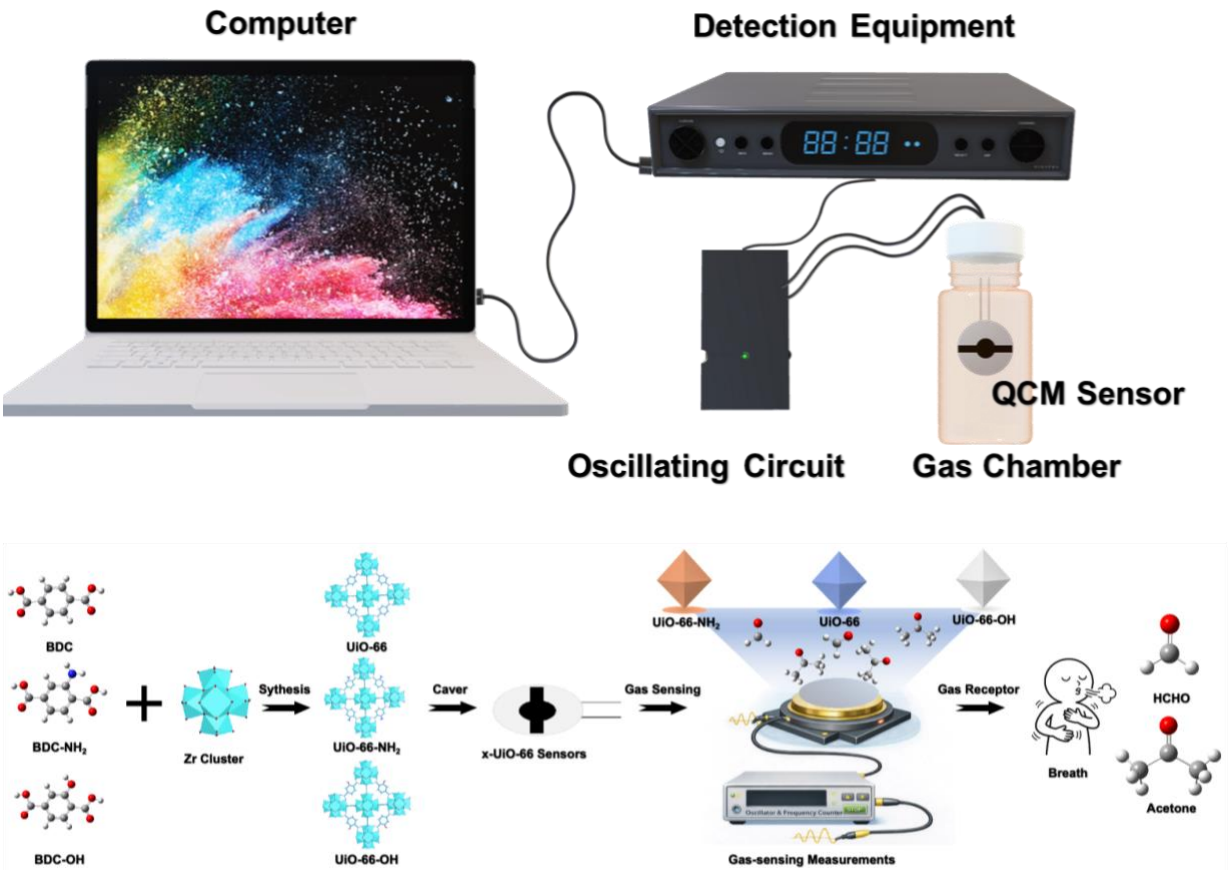

Figure S5. Schematic diagram of the gas sensor device.

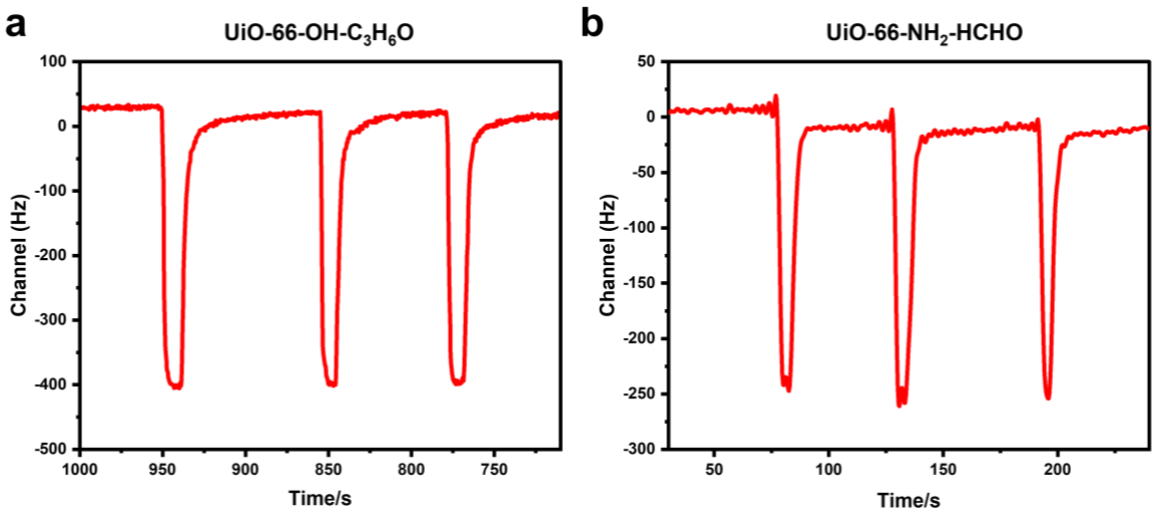

Figure S6. Cycling stability tests of UiO-66-OH–C_3H_6O and UiO-66-NH_2–HCHO over three consecutive adsorption–desorption cycles, showing stable and reproducible response signals without noticeable attenuation.

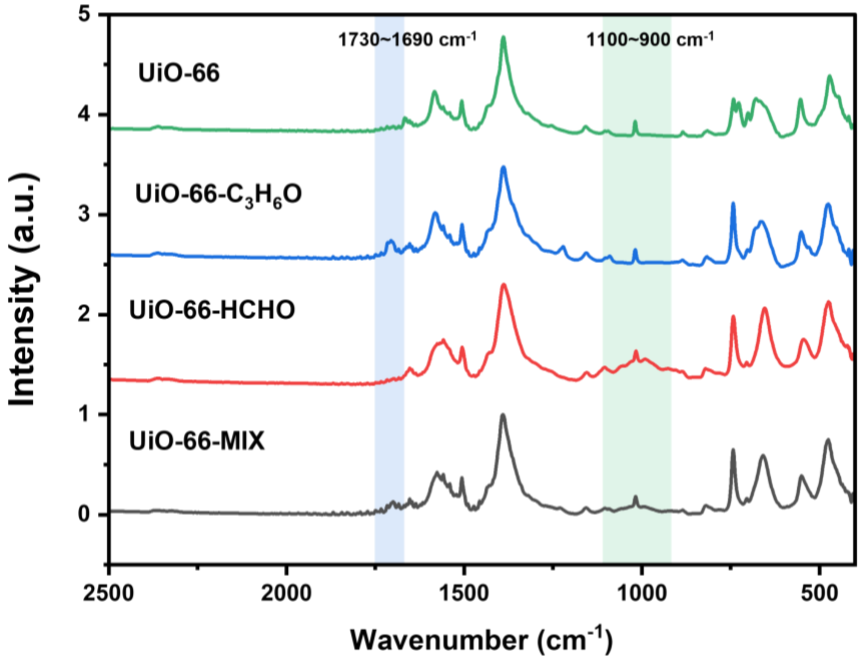

Figure S7. FTIR spectra of UiO-66 was recorded after exposure to single vapors (HCHO or C_3H_6O) and mixed vapor conditions (MIX).

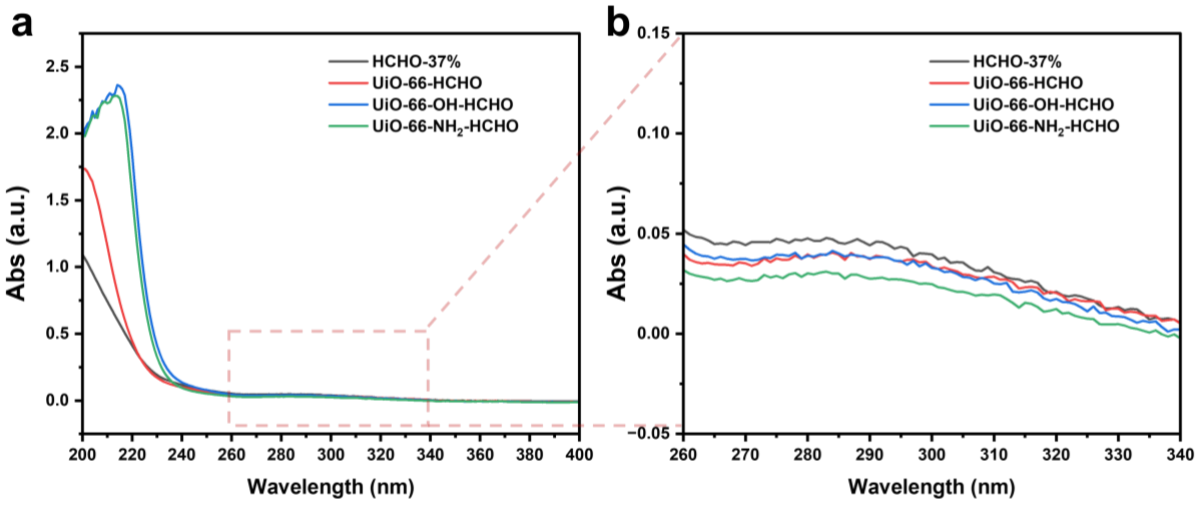

Figure S8. UV–vis absorption spectra of aqueous HCHO (37 wt%) before and after filtration through UiO-66, UiO-66-OH, and UiO-66-NH_2.

S2- Supporting Tables

Table S1. Summary Table of Computational Results.

	BDC-OH	BDC-NH_2	HCHO	Acetone	OH-HCHO	OH-Acetone	NH_2-HCHO	NH_2-Acetone
E/ Hartree	-683.853	-664.015	-114.360	-192.911	-798.229	-876.787	-778.383	-856.936
Dipole Moment/ Debye	3.846	4.795	2.2513	2.8444	7.828	5.939	8.105	8.989
Polarizability (α)/ a.u.	95.807	101.937	13.244	34.721	112.370	131.583	118.540	141.006