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Supporting information

THEORETICAL INSIGHTS INTO THE ADSORPTION AND GAS SENSING PERFORMANCE OF Fe/Cu-ADSORBED GRAPHENE

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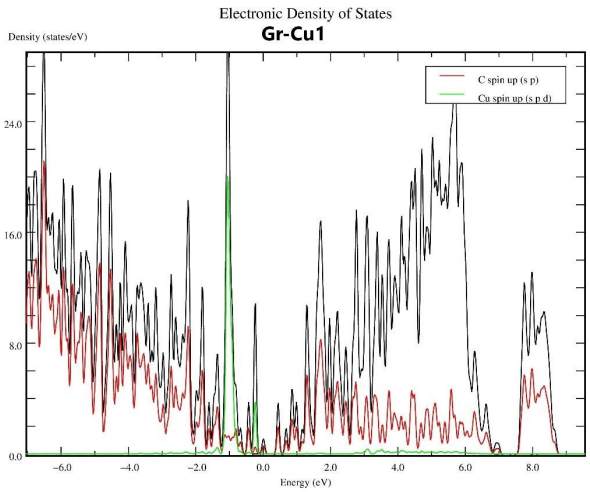
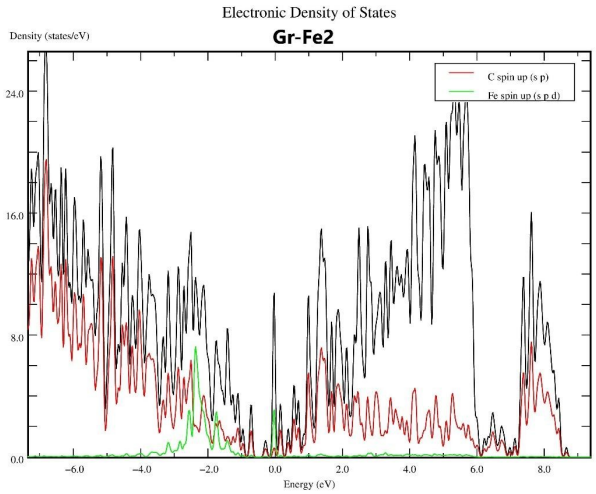
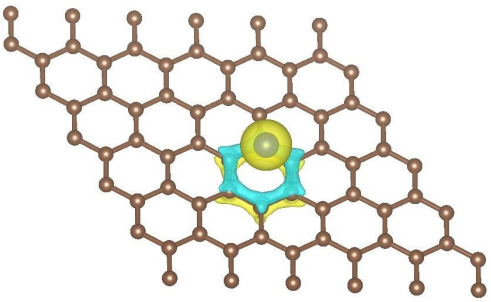
Figures:







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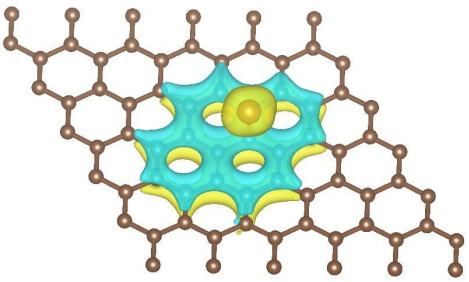

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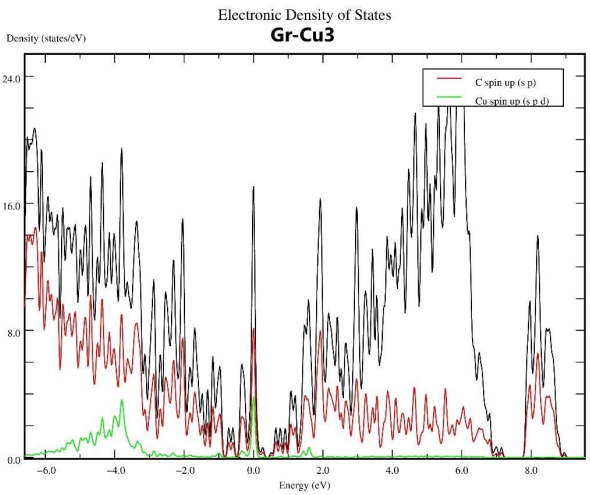

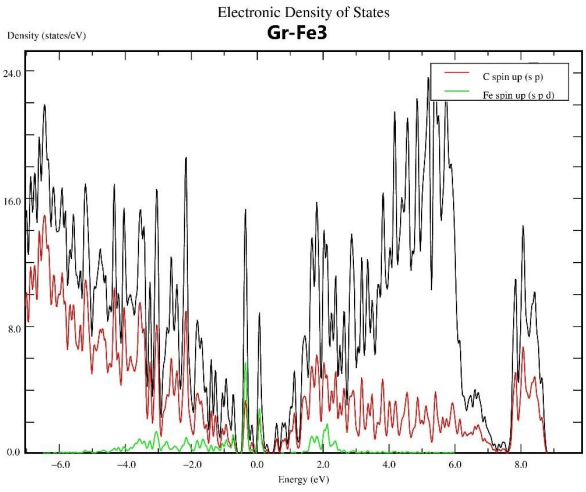

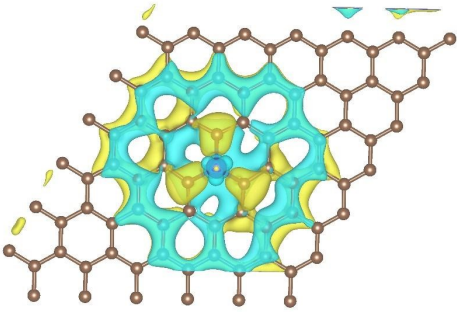

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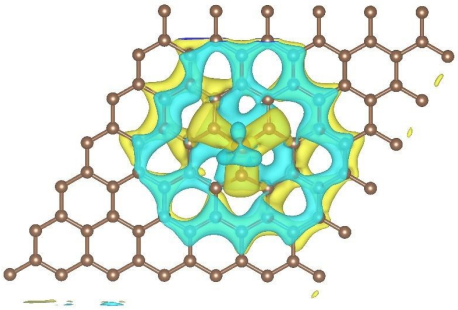
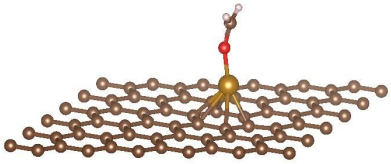


Gr-Fe3 (+1.01 e on Fe)

Figure S1. *The density of states and charge density distribution maps of* ***Gr-Fe2(3)*** *and* ***Gr-Cu1(3)*** *surfaces*



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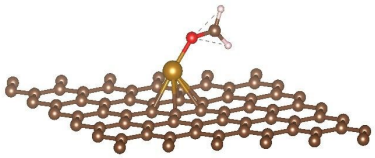

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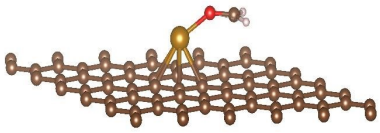

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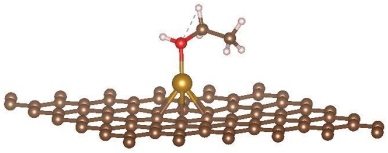

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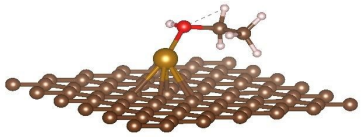

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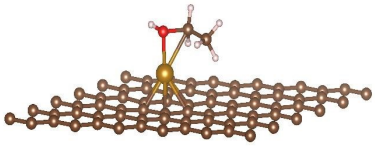

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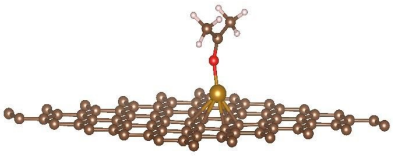

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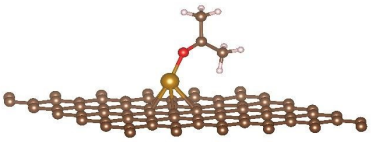

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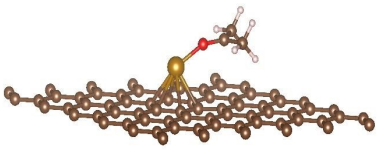

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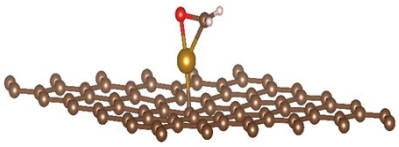

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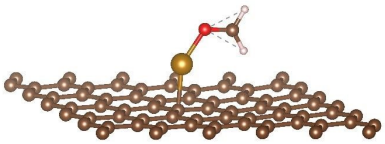

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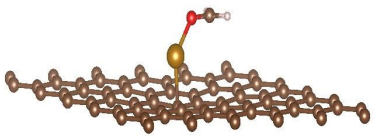

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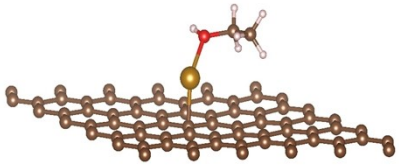

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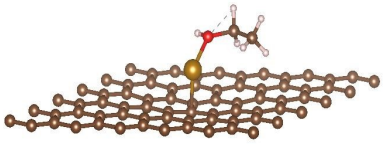

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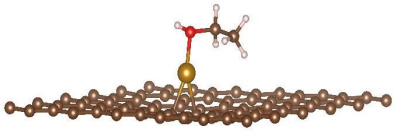

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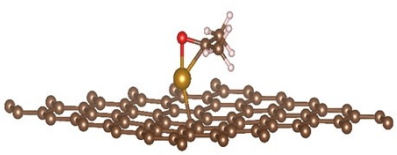

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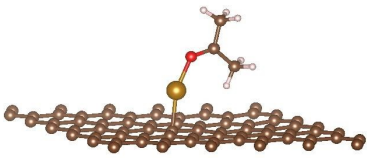

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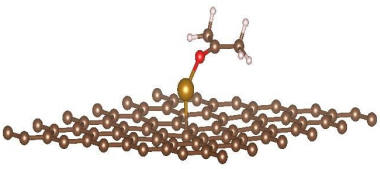

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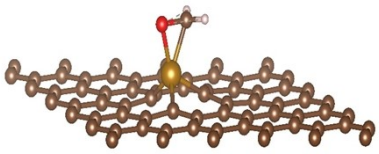

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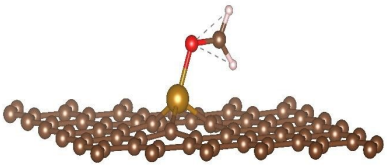

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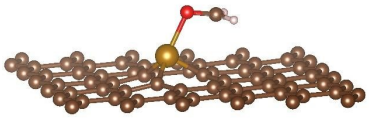

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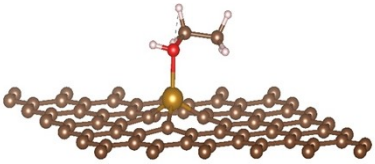

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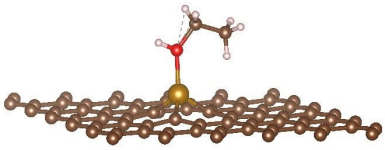

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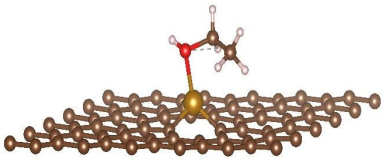

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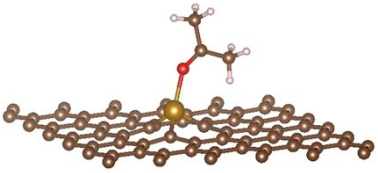

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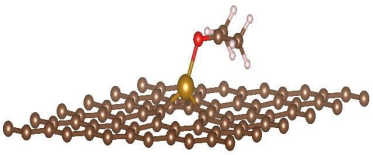

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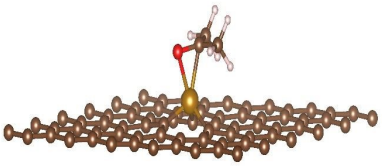

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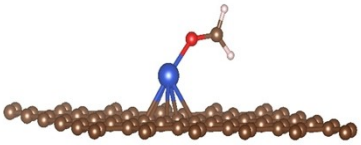

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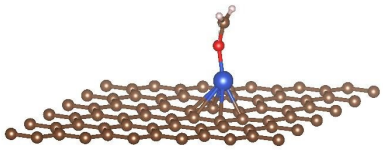

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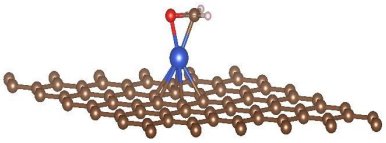

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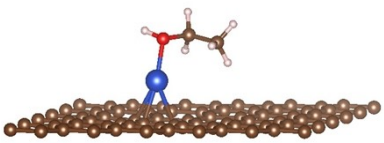

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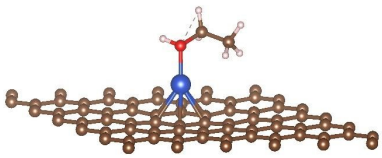

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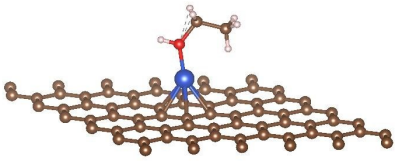

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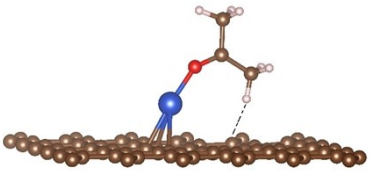

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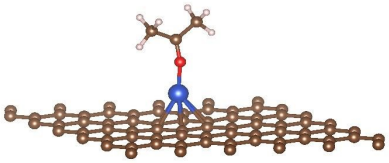

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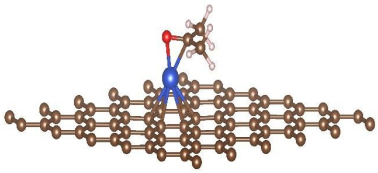

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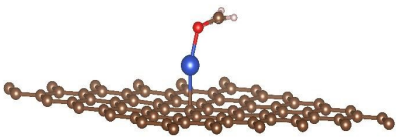

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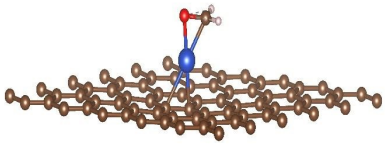

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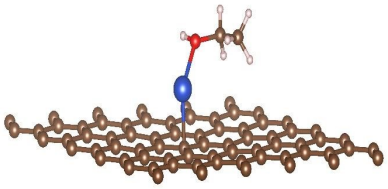

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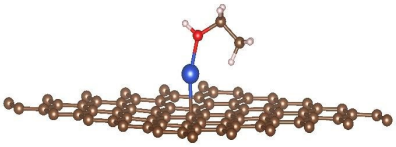

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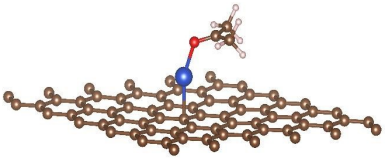

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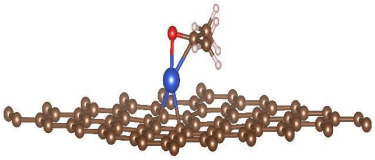

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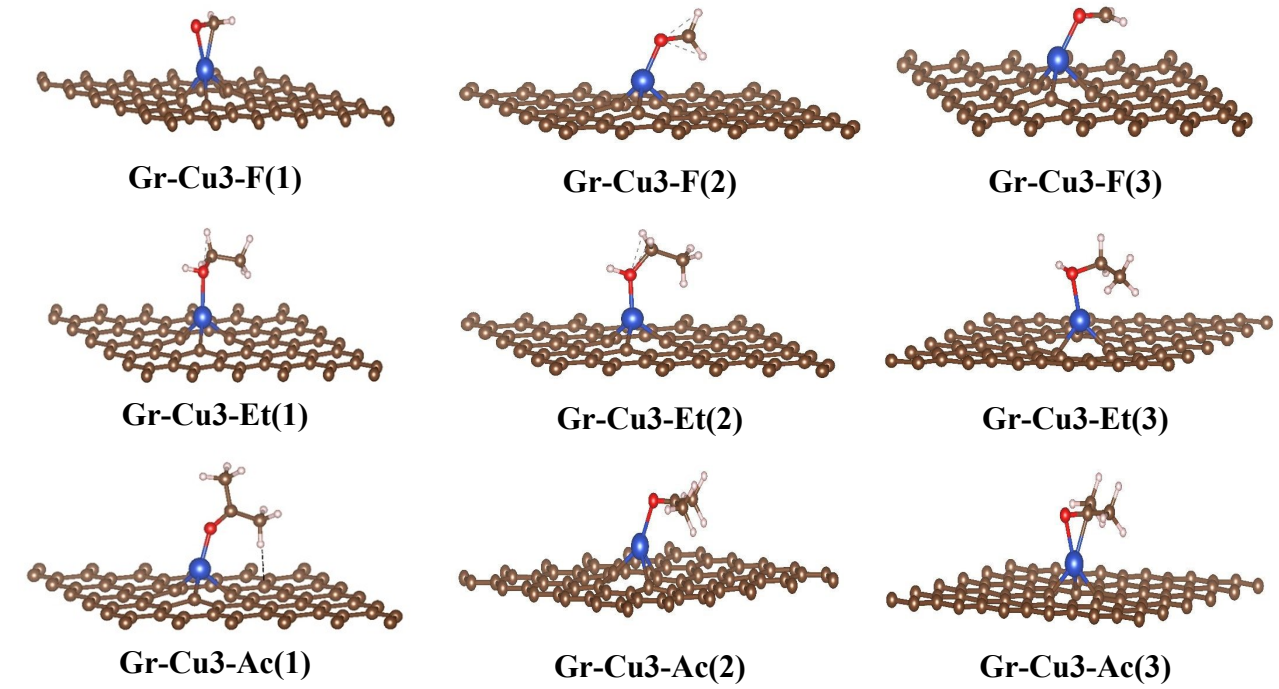


Figure S2. *The other stable complexes for* ***Gr-Mi--VOC*** *systems (M = Fe, Cu; i = 1,2,3; VOC = F (HCHO), Et (C_2H_5OH), Ac (CH_3COCH_3))*

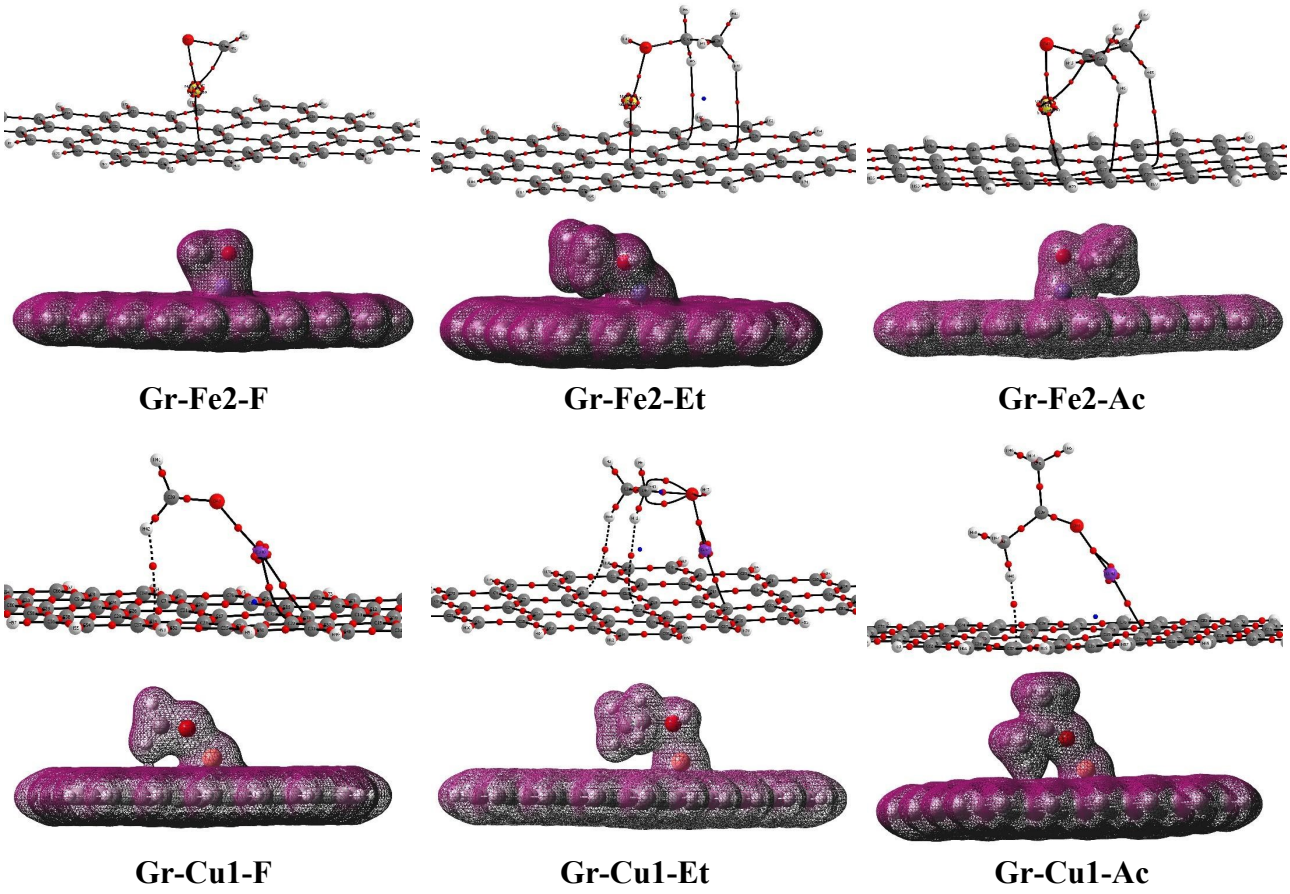


Figure S3. *The topological geometries and total electron density transfer maps for the selected configurations in* ***Gr-Fe2/Gr-Cu1--VOC*** *systems*

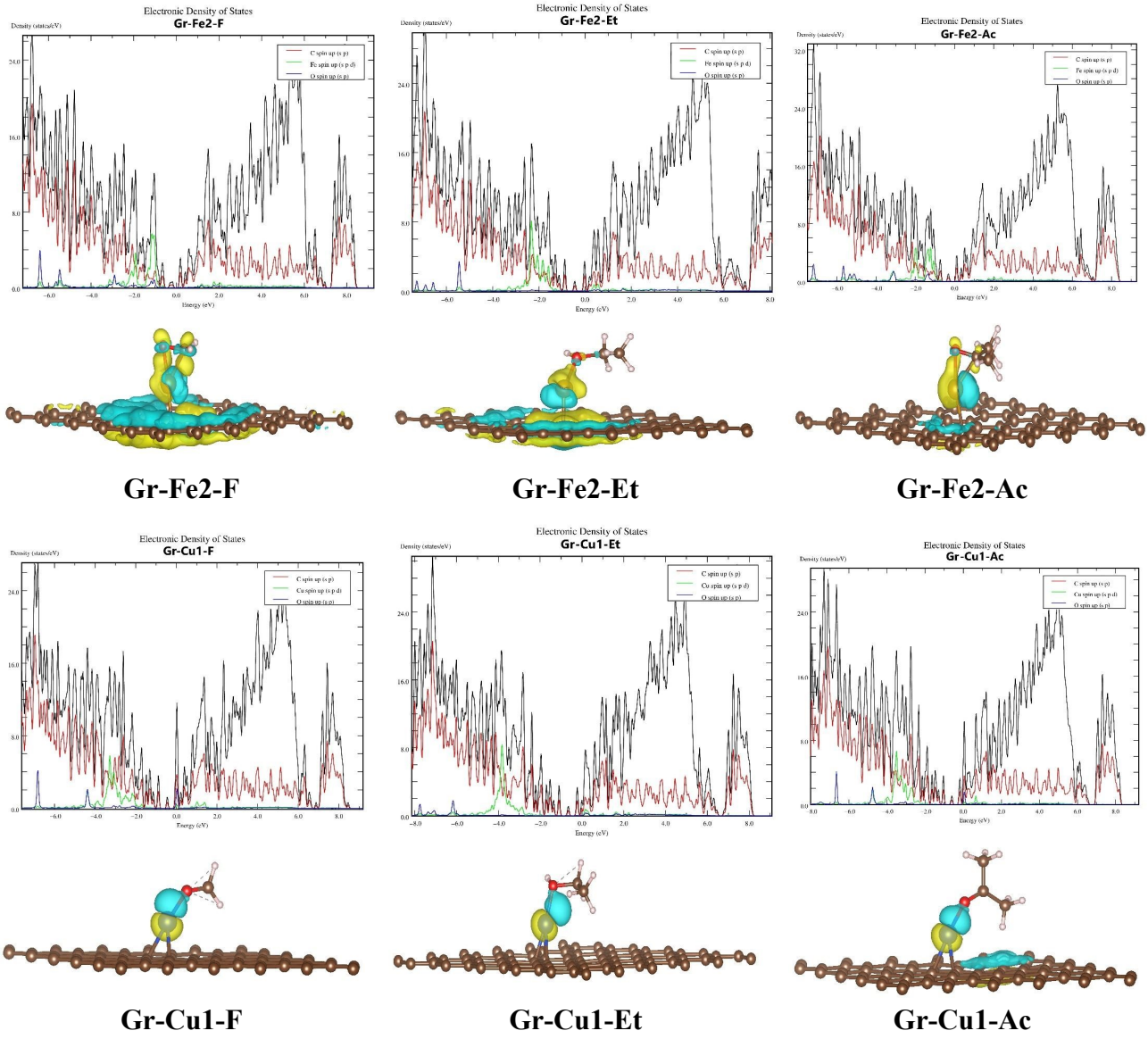
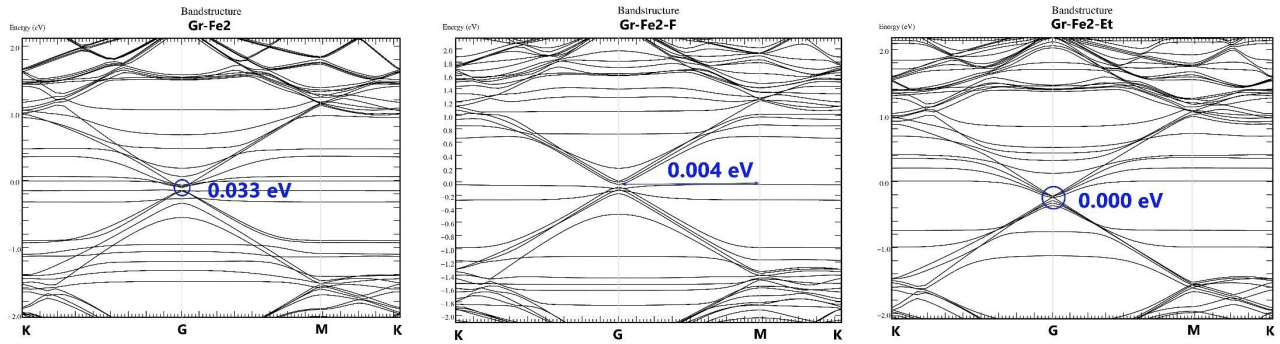


Figure S4. *The density of states and charge density difference maps of the most stable configurations for* ***Gr-Fe2****,* ***Gr-Cu1*** *surfaces*



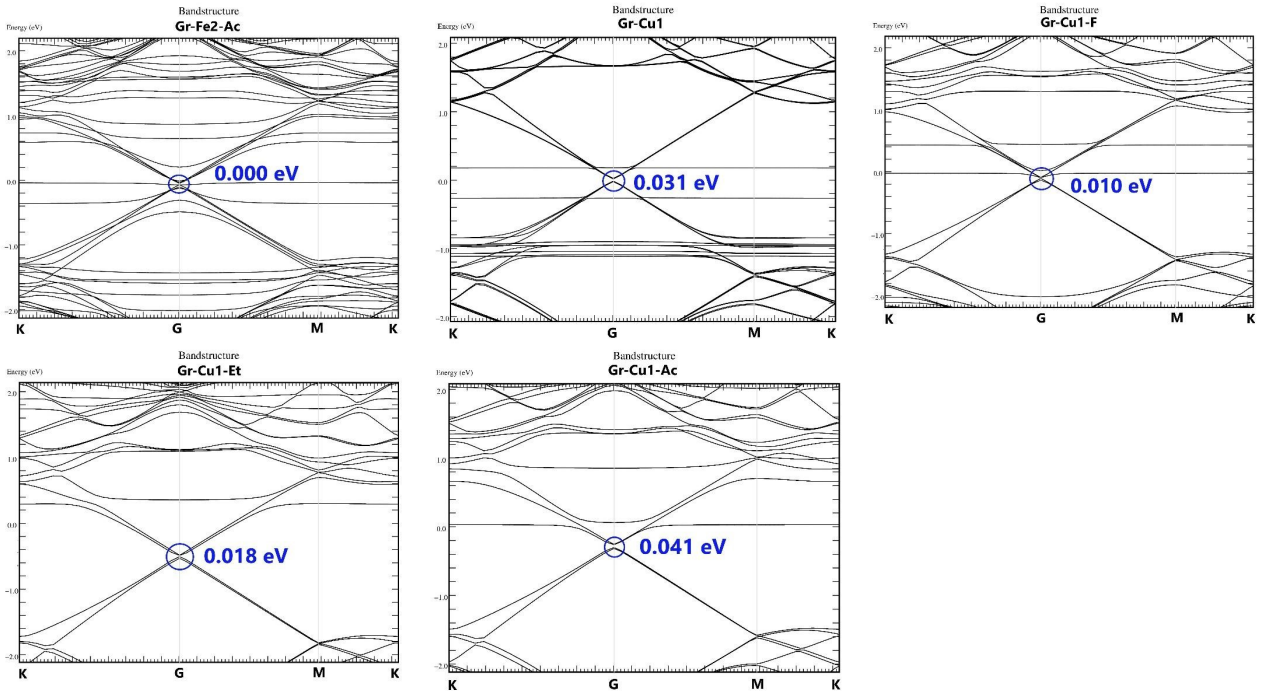


Figure S5. *The band structures of the most stable configurations in* ***Gr-Fe2/Gr-Cu1--VOC*** *systems*

Tables:

Table S1. *Adsorption energy of the other stable configurations for Fe/Cu-adsorbed graphene surfaces (Fig. S2) at the vdW-DF2 functional (in eV)*

	HCHO (F-1/2/3)	**C_2H_5OH (Et-1/2/3)**	**CH_3COCH_3 (Ac-1/2/3)**
Gr-Fe1	-1.59/-1.48/-1.23	-1.29/-1.23/-0.91	-1.48/-1.27/-1.43
Gr-Fe2	-2.33/-1.80/-1.70	-1.70/-1.52/-1.32	-2.17/-1.82/-1.84
Gr-Fe3	-1.16/-0.82/-0.65	-1.21/-1.16/-0.76	-1.12/-1.00/-0.68
Gr-Cu1	-0.70/-0.42/-0.44	-0.92/-0.69/-0.58	-0.82/-0.42/-0.53
Gr-Cu2	-0.61/-0.58	-0.71/-0.80	-0.77/-0.71
Gr-Cu3	-0.87/-0.87/-0.50	-0.72/-0.71/-0.49	-0.95/-0.79/-0.46

Table S2. *Selected parameters of AIM and NBO analyses for the stable configurations (ρ(r); $\blacklozenge^2$(ρ(r), H(r) in au, EDT in e, WBI-Wiberg bond index)*

	BCP	ρ(r)	$\blacklozenge^2$(ρ(r))	H(r)	WBI	EDT
Gr-Fe2-F	C···Fe	0.100	0.251	-0.028	0.842	0.088
Gr-Fe2-Et	O···Fe	0.118	0.590	-0.042	0.842	
	O···Fe	0.064	0.446	-0.005	0.426	0.088
Gr-Fe2-Ac	O···Fe	0.116	0.565	-0.041	0.755	0.216
Gr-Cu1-F	Cu···O	0.081	0.830	-0.005	0.210	-0.162
	H···C/π	0.008	0.035	0.002	---	
Gr-Cu1-Et	Cu···O	0.074	0.718	-0.003	0.200	0.067
	H···C/π	0.005	0.018	0.001	---	
Gr-Cu1-Ac	Cu···O	0.079	0.813	-0.004	0.202	0.056
	H···C/π	0.016	0.064	0.001	---	

Table S3. *The characteristics of gas sensing performance of* ***Gr-Fe2, Gr-Cu1*** *surfaces*

	E_g (eV)	S (%)	τ (s)		
			298K	400K	500K
Gr-Fe2-F	0.004	43.1	$2.4x10^{27}$	$2.2x10^{17}$	$3.0x10^{11}$
Gr-Fe2-Et	0.000	47.4	$5.5x10^{16}$	$2.6x10^{9}$	$1.3x10^{5}$
Gr-Fe2-Ac	0.000	47.4	$4.8x12^{14}$	$2.1x10^{15}$	$7.3x10^{9}$
Gr-Cu1-F	0.010	33.6	$9.4x10^{-3}$	$2.7x10^{-5}$	$8.8x10^{-7}$
Gr-Cu1-Et	0.018	22.4	$3.6x10^{3}$	0.4	$1.9x10^{-3}$
Gr-Cu1-Ac	0.041	21.5	72.8	$2.1x10^{-2}$	$1.8x10^{-4}$