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Supplementary Information

Theoretical insight into the interaction on Ni and Cu surfaces for HMF hydrogenation: a density functional theory study

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1. Optimization of isolated molecules

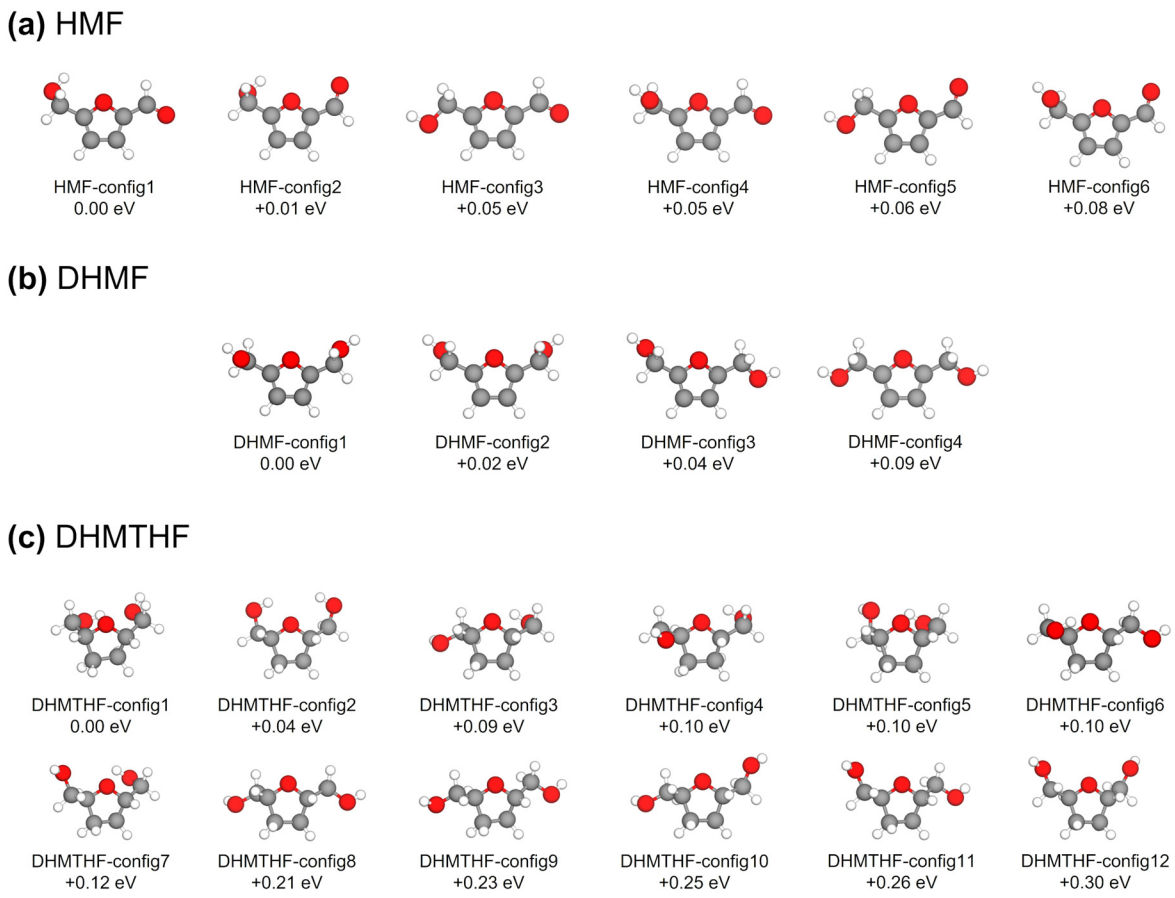


Figure S1 The possible configurations of molecules optimized by PAWPBE-D3. The energy of most stable configuration (config1) is used as the reference for each molecule.

2. Adsorption on Ni and Cu surfaces

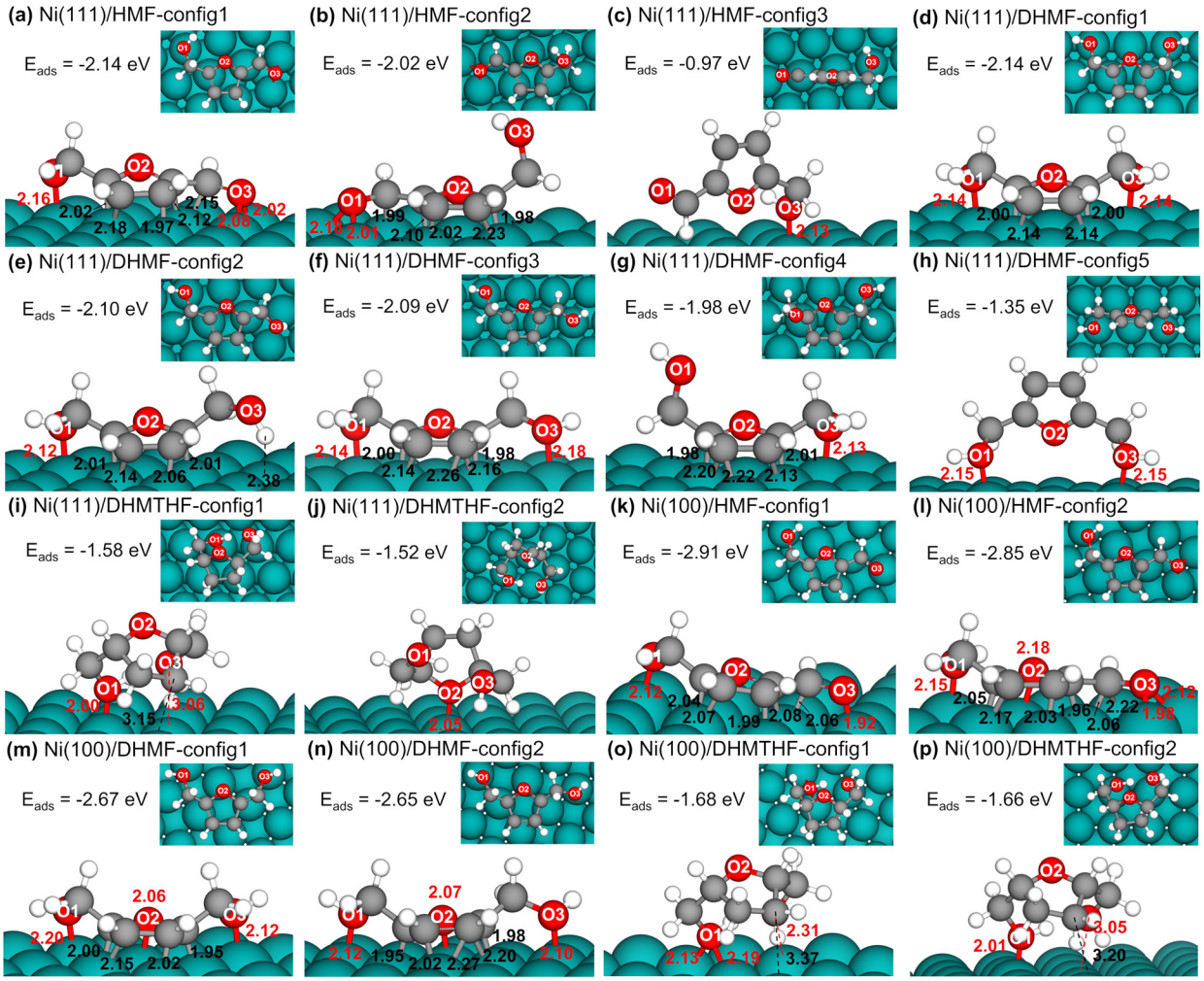


Figure S2 The optimized adsorption configurations of HMF, DHMF and DHMTHF on Ni surfaces

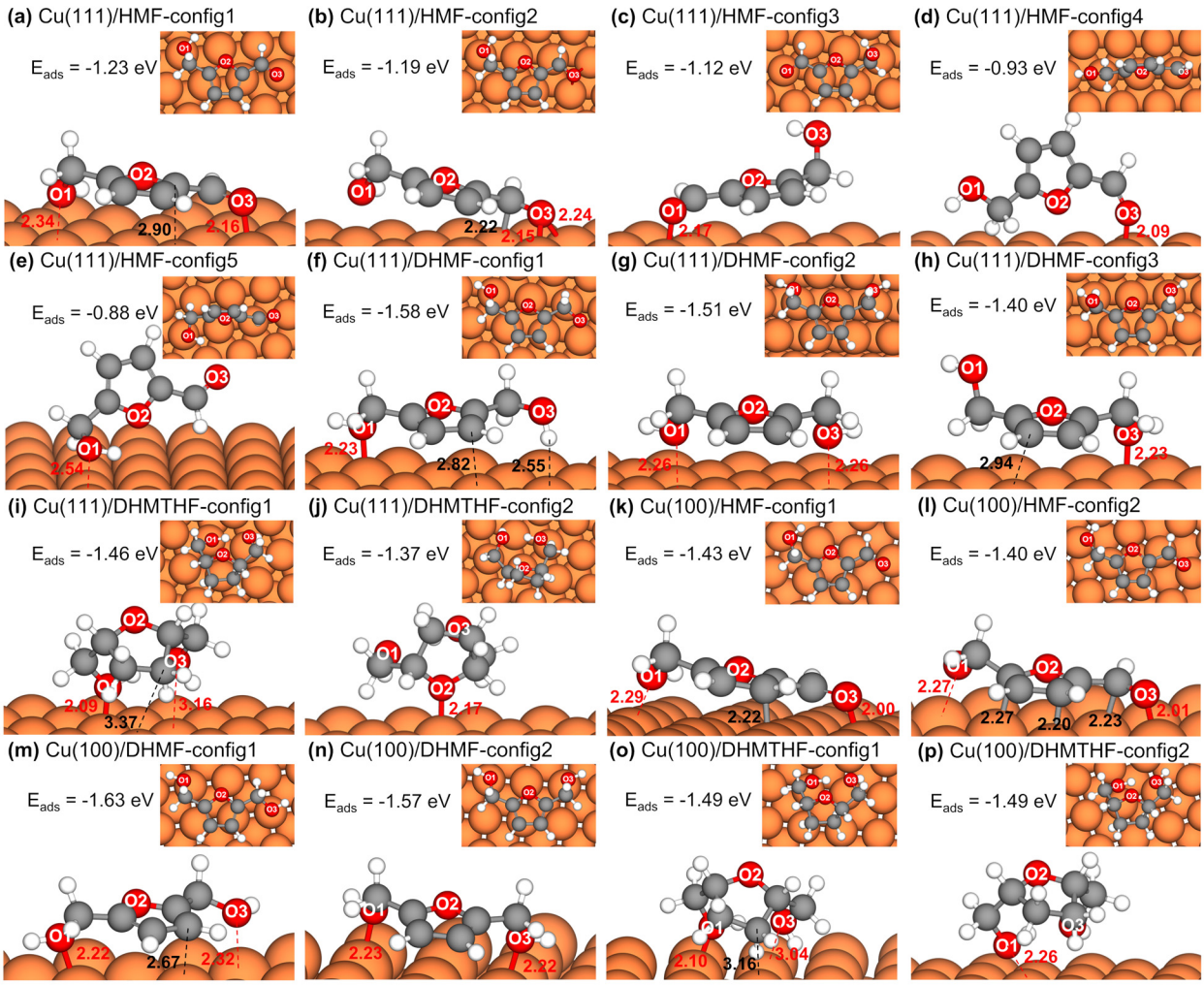


Figure S3 The optimized adsorption configurations of HMF, DHMF and DHMTHF on Cu surfaces

3. Charge analysis

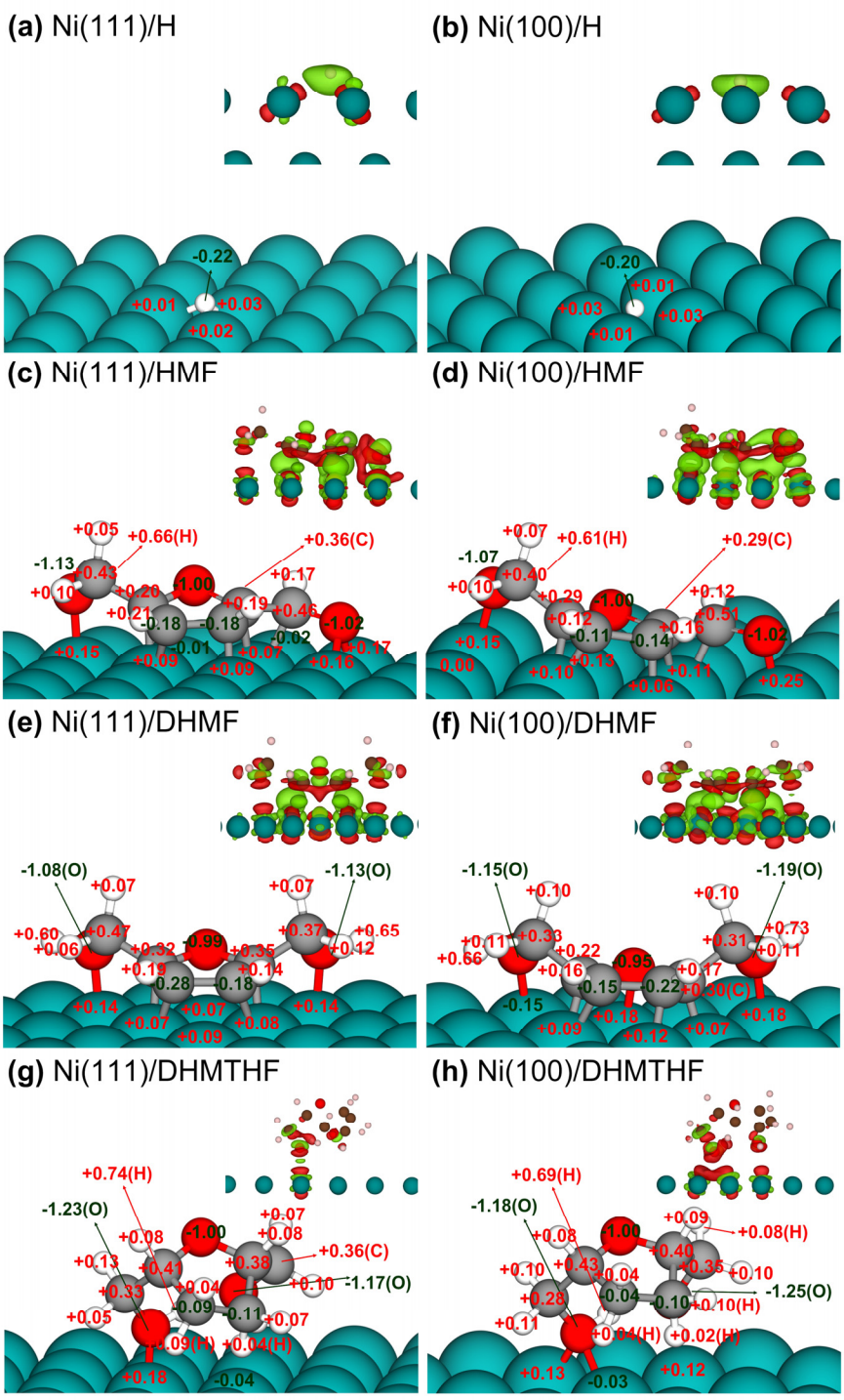


Figure S4. The Bader charge change of selected atoms and charge density difference (presented in the top right panel) of (a-b) H, (c-d) HMF, (e-f) DHMF, and (g-h) DHMTHF adsorptions on Ni(111) and Ni(100) surfaces. The green and red regions with isosurface of ±0.005 |e|/Å^3 represent charge accumulation and depletion, respectively.

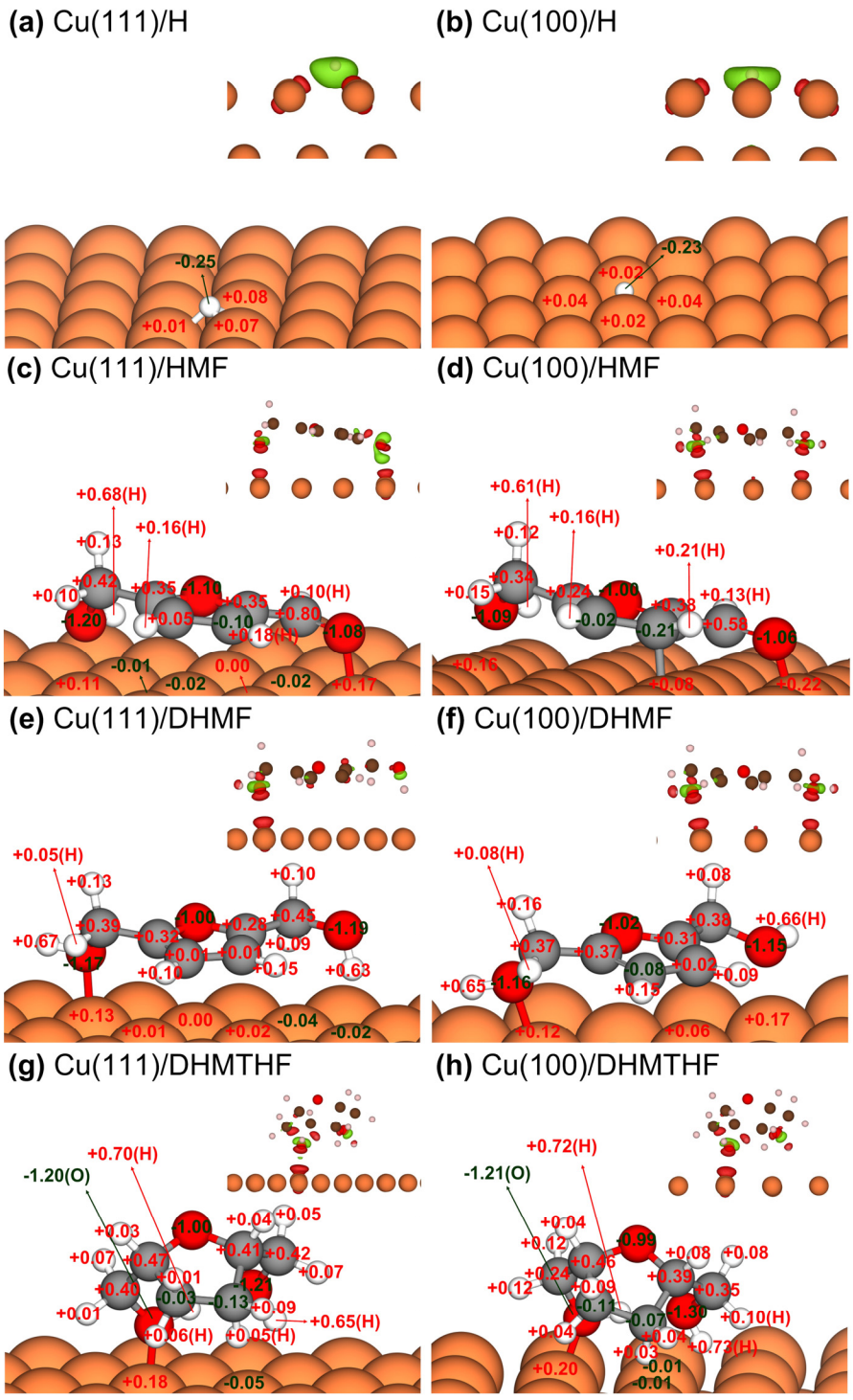
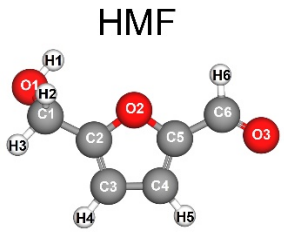


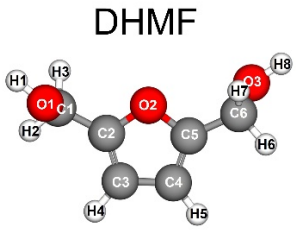
Figure S5. The Bader charge change of selected atoms and charge density difference (presented in the top right panel) of (a-b) H, (c-d) HMF, (e-f) DHMF, and (g-h) DHMTHF adsorptions on Cu(111) and Cu(100) surfaces. The green and red regions with isosurface of ±0.005 |e|/Å^3 represent charge accumulation and depletion, respectively.

Table S1 The Bader charge difference (in |e|) of the adsorbed HMF compared with the pre-adsorbed HMF.



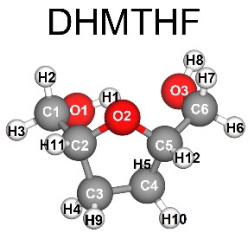
	Ni(111)	Ni(100)	Cu(111)	Cu(100)
C1	0.0312	-0.0068	0.0136	-0.0618
C2	-0.0566	0.0271	0.0874	-0.0143
C3	-0.2850	-0.2097	-0.0551	-0.1176
C4	-0.1960	-0.1532	-0.1199	-0.2322
C5	0.1378	0.0633	0.1270	0.1533
C6	-0.5455	-0.4913	-0.2032	-0.4206
O1	-0.0424	0.0114	-0.1103	-0.0034
O2	0.0282	0.0454	-0.0754	0.0254
O3	0.0092	0.0092	-0.0442	-0.0328
H1	0.0447	-0.0053	0.0696	-0.0080
H2	-0.0432	-0.0209	0.0323	0.0263
H3	-0.0303	-0.0311	-0.0296	0.0134
H4	0.1117	0.0167	0.0638	0.0573
H5	0.0333	0.0089	0.0321	0.0528
H6	0.1220	0.0744	0.0551	0.0873

Table S2 The Bader charge difference (in |e|) of the adsorbed DHMF compared with the pre-adsorbed DHMF.



	Ni(111)	Ni(100)	Cu(111)	Cu(100)
C1	0.0922	-0.0542	0.0108	-0.0069
C2	-0.0209	-0.1155	-0.0212	-0.0112
C3	-0.4156	-0.2894	-0.1257	-0.2162
C4	-0.1547	-0.2019	0.0278	0.0433
C5	0.0793	0.0258	0.0045	0.0797
C6	-0.0126	-0.0730	0.0657	-0.0051
O1	0.0546	-0.0198	-0.0391	-0.0259
O2	0.0473	0.0847	0.0398	0.0131
O3	-0.0051	-0.0671	-0.0736	-0.0274
H1	-0.0373	0.0246	0.0311	0.0106
H2	-0.0063	0.0257	-0.0317	-0.0044
H3	-0.0234	0.0257	-0.0518	-0.0832
H4	0.1350	0.1019	0.0423	0.0952
H5	-0.0041	0.0212	0.0046	-0.0537
H6	0.0513	0.0369	0.0258	0.0048
H7	-0.0237	0.0091	-0.0093	0.0134
H8	0.0159	0.0900	-0.0071	0.0211

Table S3 The Bader charge difference (in |e|) of the adsorbed DHMTHF compared with free DHMTHF molecules.



	Ni(111)	Ni(100)	Cu(111)	Cu(100)
C1	-0.1024	-0.1559	-0.0298	-0.1892
C2	-0.0188	0.0042	0.0417	0.0356
C3	-0.0876	-0.0376	-0.0340	-0.1088
C4	-0.1070	-0.0900	-0.1270	-0.0606
C5	0.0015	0.0155	0.0307	0.0054
C6	-0.0945	-0.1035	-0.0345	-0.0991
O1	0.0825	0.1304	0.1117	0.0962
O2	0.0170	-0.0097	0.0018	0.0123
O3	-0.0533	-0.1324	-0.0938	-0.1856
H1	-0.0458	-0.0995	-0.0867	-0.0660
H2	0.0631	0.0357	0.0061	0.0582
H3	0.0162	0.0764	-0.0068	0.0834
H4	0.0428	-0.0039	0.0140	-0.0058
H5	-0.0092	-0.0294	-0.0047	-0.0258
H6	0.0382	0.0184	0.0120	0.0385
H7	0.0786	0.0873	0.0625	0.0838
H8	0.0068	0.0921	0.0420	0.1259
H9	0.0586	0.0561	0.0217	0.1057
H10	0.0324	0.0634	0.0519	0.0022
H11	0.0652	0.0691	0.0027	0.0242
H12	0.0253	0.0330	-0.0154	0.0211

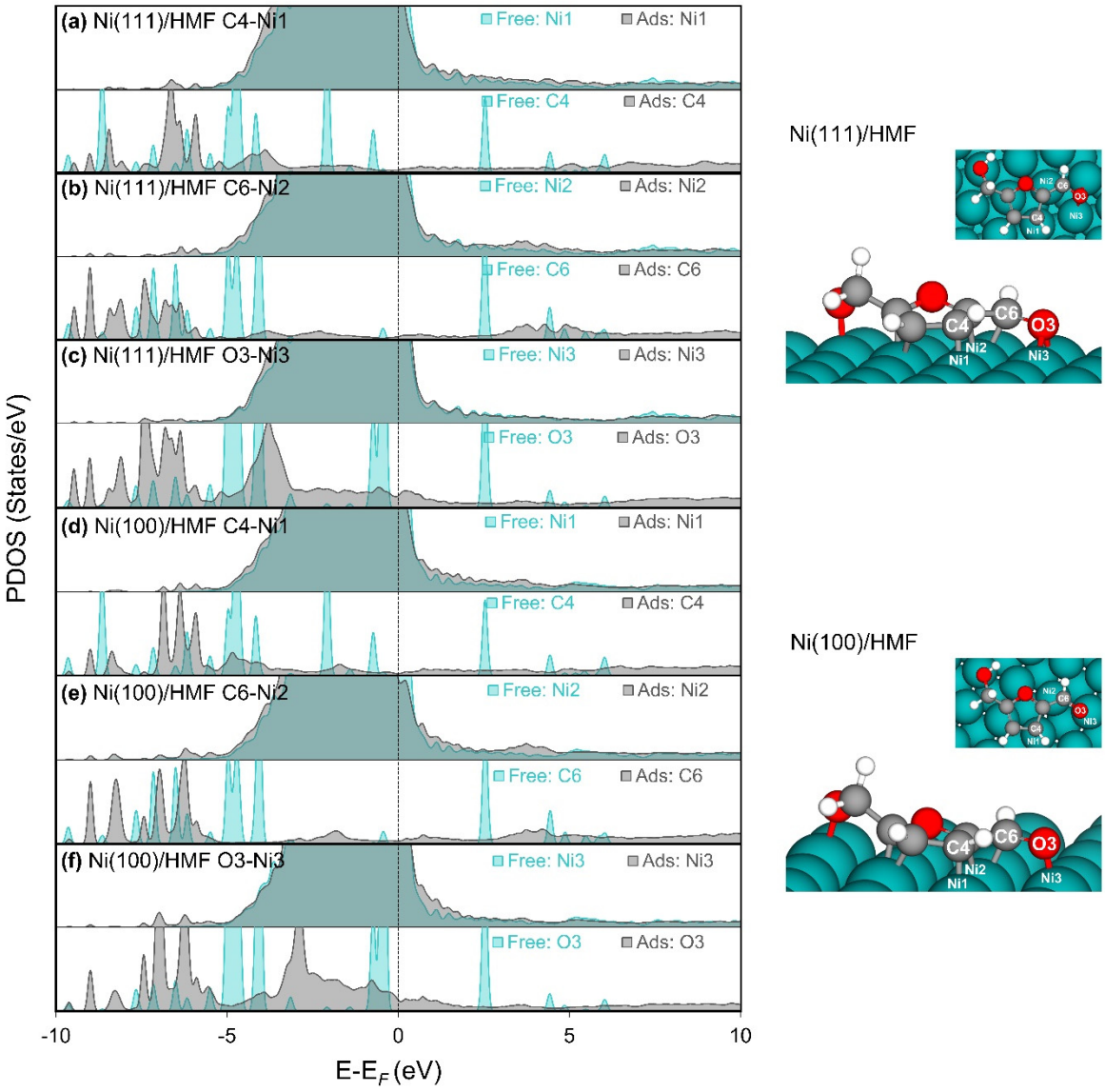


Figure S6 PDOS peaks of PDOS plots of selected atoms of (a-c) HMF adsorption on Ni(111) of the relevant configuration on the right panel and (d-f) HMF adsorption on Ni(100) surfaces of the relevant configuration on the right panel. The 3*d*-states of Cu and 2*p*-states of C and O are compared between pre-adsorption and adsorption processes.

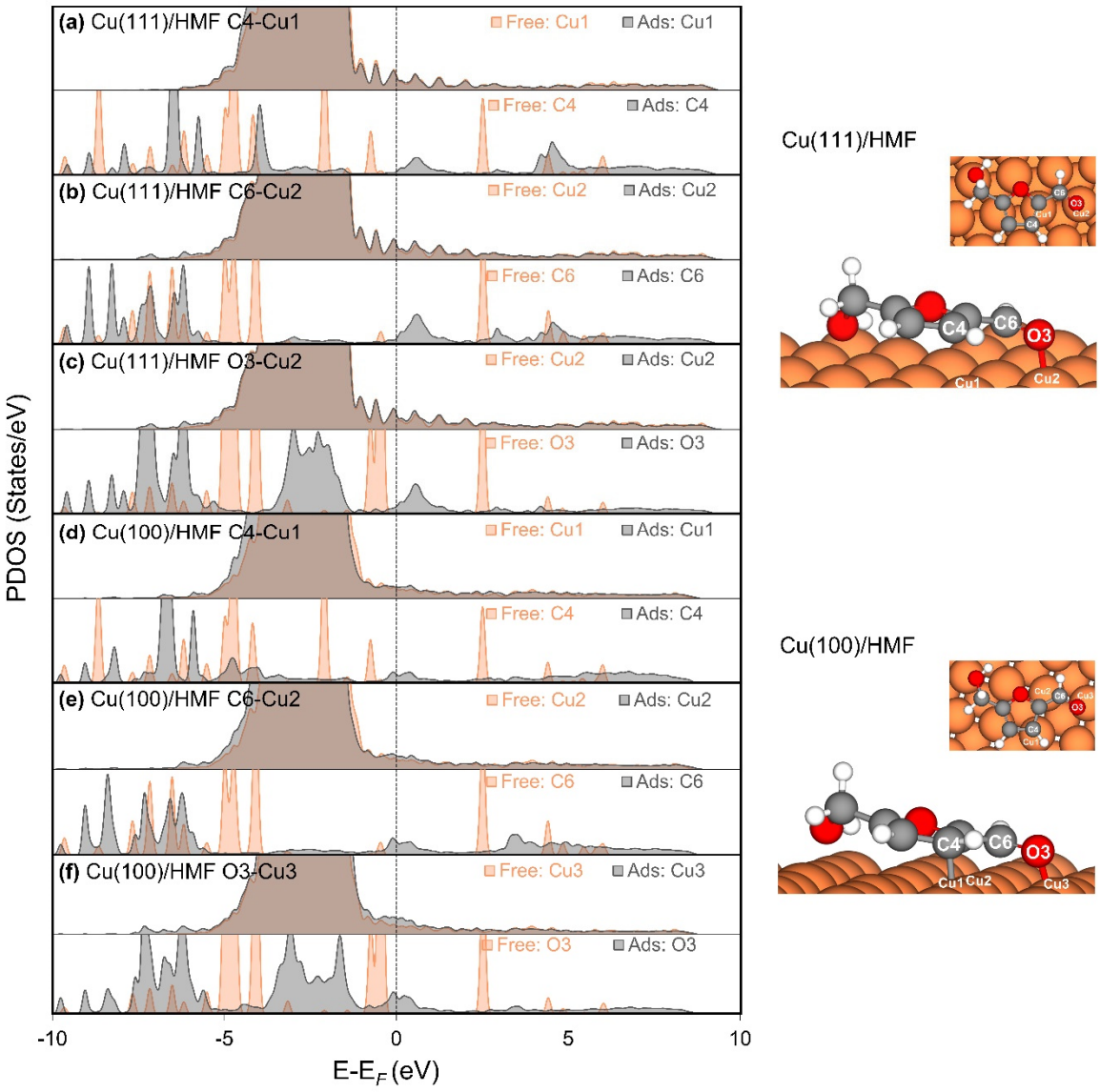


Figure S7 PDOS peaks of PDOS plots of selected atoms of (a-c) HMF adsorption on Cu(111) of the relevant configuration on the right panel and (d-f) HMF adsorption on Cu(100) surfaces of the relevant configuration on the right panel. The 3*d*-states of Cu and 2*p*-states of C and O are compared between pre-adsorption and adsorption processes.