Support Information

Can Hammett indicators Accurately Measure the Acidity of Zeolite Catalysts with Confined Space? Insights into the Mechanism of Coloration

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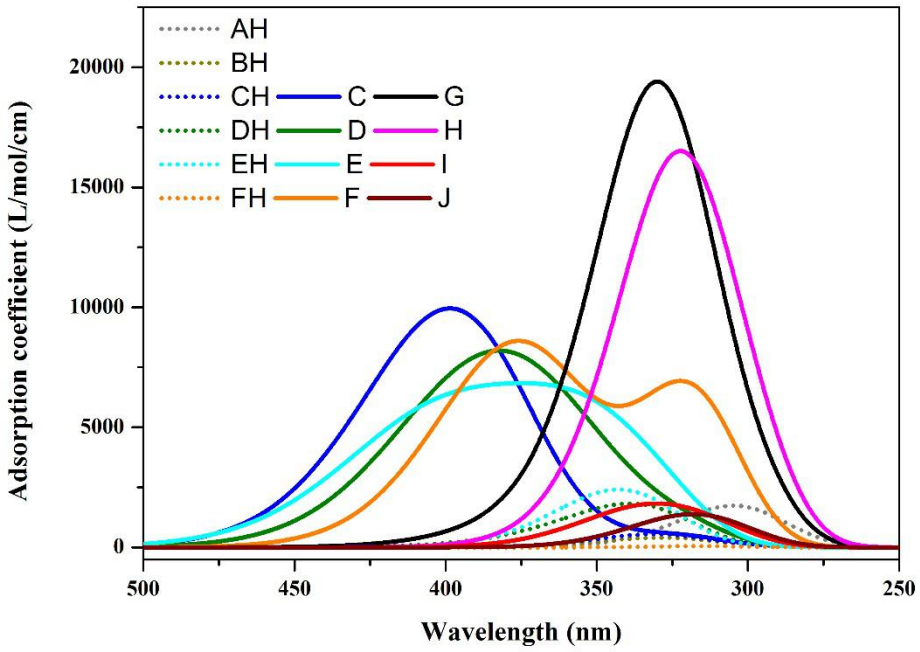

Figure 1. TDDFT predicted UV-vis spectrums of Hammett indicators in H-ZSM-5 zeolite.

Table S1. The calculated HOMO-LUMO gap (eV), maximum adsorption wavelength (nm) and their transition contribution of Hammett indicators (X) and its cationic form (HX^+) in H-ZSM-5 at the level of B3LYP/6-31G(d,p).

TYPE		H-ZSM-5						
		X			HX^+		Wave length	Contribution $_{HOMO→LUMO}$
		Gap	**ΔE_{ad}[a]**	**r(O-H)**	**Gap**	**r(O-H)**		
	A	-		-	4.43	2.197	-	-
	B	-		-	4.03	2.132	-	-
	C	3.68	-133.68	0.974	4.06	2.110	398	98%
Ⅰ	D	3.83	-79.87	0.974	3.81	1.912	394	90%
	E	3.76	-68.66	0.974	3.94	1.692	407	93%
	F	3.91	-165.77	0.974	3.61	1.990	377	98%
	G	4.04	-161.50	1.031	-	-	-	-
Ⅱ	H	4.17	-152.51	1.025	-	-	-	-
	I	4.37	-141.42	1.022	-	-	-	-
	J	4.67	-140.62	0.989	-	-	-	-

[a]ΔE_{ad} is the adsorption energy (kJ/mol) of Hammett indicators in H-ZSM-5.

Table S2. The HOMO-LUMO gap (eV), O-H distances (Å), maximum absorption wavelength (L) (nm) and their transition contribution of Hammett indicators (A-J) in the 12MR and side pocket of H-MOR at the level of B3LYP/6-31G(d,p).*

TYPE		12MR			Side-pocket				
		Gap	$\Delta \mathbf{E}_{ad}$[d]	r(O-H)	Gap	$\Delta \mathbf{E}_{ad}$[d]	r(O-H)	L	Contribution
I	A	4.79	-	1.639	-	-	-	-	-
	B	4.34	-	1.631	-	-	-	-	-
	C	4.42	-	1.620	-	-	-	-	-
	D	4.03	-	1.620	-	-	-	-	-
	E	3.92	-	1.584	-	-	-	-	-
	F	3.89	-	1.557	-	-	-	-	-
II	G	4.20	-190.8	1.052	3.95	-104.0	1.050	388	86%[a]+3%[b]
	H	4.32	-174.9	1.040	4.00	-87.6	1.041	417	93%[a]
	I	4.32	-193.3	1.031	3.88	-109.1	1.038	404	36%[a]+42%[b]+9%[c]
	J	4.43	-174.2	1.026	3.93	-82.3	1.030	404	33%[a]+50%[b]

*Transition contributions of [a]HOMO→LUMO, [b]HOMO-1→LUMO, [c]HOMO→LUMO+1. [d]$\Delta \mathbf{E}_{ad}$ is the adsorption energy of Hammett indicators in 12MR and side-pocket of H-MOR.

Table S3. The HOMO-LUMO gap (eV), maximum adsorption wavelength (nm) and their transition contribution of Hammett indicators (X=C-F) and its cationic form (HX+) in the HY.

X	Clusters	pKa	Gap	ΔE_{ad}[f]	r(O-H)	Wavelength (nm)		Contribution
						HY	Free	
C	HY	-5.48	4.42	-	1.511	321	400	-
D	HY	-8.37	4.34	-120.88	1.006	344	393	82%[a] +7%[b]
E	HY		4.26	-111.38	0.998	348	391	81%[a] +7%[b]
E	HY-A	-9.71	4.00	-153.97	1.003	365	391	93%[a]
E	HY-B		4.42	-147.28	1.008	354	391	13%[a]+49%[b]+19%[e]
E	HY-C		4.40	-149.37	1.014	350	391	21%[a]+43%[b]+17%[e]
F	HY		4.42	-127.74	1.012	337	381	79%[a]+10%[c]
F	HY-A	-10.10	4.03	-109.70	0.987	366	381	96%[a]
F	HY-B		4.31	-120.62	1.000	343	381	93%[a]
F	HY-C		4.32	-119.66	0.999	346	381	88%[a]+5%[d]

Transition contributions of [a]HOMO → LUMO, [b]HOMO → LUMO+1; [c]HOMO-3 → LUMO; [d]HOMO-4 → LUMO; [e]HOMO-2 → LUMO+1; [f]ΔE_{ad} is the adsorption energy (kJ/mol) of Hammett indicators in HY.