Simultaneous recognition of dopamine and uric acid in the real sample through highly sensitive new electrode fabricated by ZnO/carbon quantum dots: Bio-imaging and theoretical studies

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Supplementary materials

Table S1. XRD data of different of the samples.

Crystal Planes	Difraction peaks *2θ*[°]			
	ZnO	ZnO-CQDs	JCPDS 36-1451	Δ2θ
(100)	31.78	31.78	31.77	0.01
(002)	34.43	34.43	34.44	-0.01
(101)	36.25	36.27	36.25	0
(102)	47.58	47.48	47.53	0.05
(110)	56.6	56.62	56.6	0
(113)	62.87	62.85	62.6	0.27
(200)	66.45	66.39	66.38	0.07
(112)	67.95	67.95	67.96	-0.01
(201)	69.08	69.08	69.1	-0.02
(004)	72.66	72.52	72.56	0.1
(202)	76.99	76.89	76.95	0.04

Table S2. Elemental composition of samples.

Element	CQDs		ZnO		ZnO/CQDs	
	%W	%T	%W	%T	%W	%T
Zn	-	-	66.96	33.16	59.57	21.89
C	56.84	63.4	-	-	34.85	69.72
O	36.39	30.47	33.04	66.84	5.58	8.38
N	6.18	5.92	-	-	-	-
Total	100	100	100	100	100	100

Table S3. Bond lengths (Å) and bond angles (°) resulted in different spin states for [ZnO wurtzite, ZnO wurtzite-dopamine and ZnO wurtzite-Uric acid], using Functional B3LYP/DGDZVP level of theory.

	DGDZVP					
Bond length ligand	**Dopamine (L^1)**	**Uric acid (L^2)**	**Bond length complexes (Å)**	**ZnO wurtzite**	**[ZnO wurtzite-Dopamine] in the corner of ZnO surface**	**[ZnO wurtzite-uric acid at the lateral plane of ZnO surface**
O1-C1		1.219	Zn1-Zn3	2.625	2.621	2.819
C1-N1	1.466	1.382	Zn1-O1	2.012	1.972	1.907
C1-N2	-	1.426	Zn1-O2	2.012	-	2.118
			Zn1-Zn2	2.616	-	-
			Zn2-Zn3	2.626	-	-
			Zn2-O1	2.014	-	-
			Zn2-O2	2.014	-	-
			Zn3-O1	2.007	-	-
			Zn3-O2	2.007	-	-
N1-H1	1.012	1.011	Zn1-H1	-	-	2.810
N2-H2	1.012	1.012	Zn1-O3	-	-	2.363
C1-H3	1.097		Zn1-C4	-	-	2.887
C1-H4	1.097		Zn1-C2	-	-	2.734
			Zn1-N1	-	-	1.973
			Zn2-O1	-	1.948	
			Zn2-Zn3	-	2.219	
			Zn2-O2	-	2.271	
			Zn3-O2	-	1.927	
			O2-N1	-	1.424	
			O2-H1	-	1.950	
			O2-C1	-	2.348	
			O2-H2	-	2.538	
			O2-H3	-	2.637	
			Bond Angle (o)			
			O2-Zn2-O1	82.2	82.3	
			O2-Zn3-O1	82.5	92.4	
			Zn1-Zn2-O1	49.4	140.7	
			O2-N1-H1		104.6	
			O2-N1-C1		108.8	
			O2-C1-H2		86.8	
			O2-C1-H2		92.7	
			O2-C1-C2		145.0	
			Zn2-O2-N1		138.2	
			Zn2-O2-c1		111.2	
			Zn2-O2-H1		119.5	

			Zn3-O2-N1		133.9	
			Zn3-O2-C1		142.0	
			Zn3-O2-H1		142.2	
			Zn3-O2-H2		150.0	
			Zn3-O2-H3		118.3	
			Zn1-O1-Zn2	81.0		167.8
			Zn1-Zn3-Zn2	60.1		92.6
			Zn1-O2-Zn3	81.6		88.4
			Zn1-H1-Zn3			62.2
			Zn1-O2-H1			127.0
			Zn1-N1-C1			145.0
			Zn1-N1-C2			107.7
			Zn1-C2-C4			81.7
			Zn1-C2-C3			155.3
			Zn1-C4-N3			177.0
			Zn1-O3-C4			101.4
			H1-Zn1-O3			87.4
			H1-Zn1-C4			97.4
			H1-Zn1-C2			106.7
			H1-Zn1-N1			111.8
			O2-Zn1-O3	82.3		101.2
			O2-Zn1-C4			113.3
			O2-Zn1-C2			121.6
			O2-Zn1-N1			121.2
			Zn3-Zn1-O3	49.1		111.5
			Zn3-Zn1-C4			135.7
			Zn3-Zn1-C2			160.2
			Zn3-Zn1-N1			159.0
			O1-Zn1-N1			144.4
			Zn1-O2-Zn3	81.5		

Table S4. Mulliken charges of L^1 and L^2 and its complexes of ZnO wurtzite with. Functional B3LYP/DGDZVP basis set.

Atoms	**Dopamine (DA)**	**Uric acid (UA)**	**Atoms**	**ZnO wurtzite**	**[ZnO wurtzite-Dopamine] in the perpendicular position of ZnO surface**	**[ZnO wurtzite- uric acid at the corner orientation of ZnO surface**
N1	-0.707	-0.459	**Zn1**	0.656	0.223	1.267
C1	-0.317	0.303	**Zn2**	0.656	0.395	0.476
C2	-0.517	0.106	**Zn3**	0.656	0.605	0.758
C3	0.318	0.398	**O1**	-0.984	-0.822	-1.166
C4	0.241	0.314	**O2**	-0.984	-0.600	-1.098
C5	-0.378	0.377	**O3**		-0.610	-0.607
C6	-0.282		**O4**		-0.560	-0.584
C7	0.293		**O5**			-0.803
C8	-0.326		**N1**		-0.245	-0.903
O1	-0.610	-0.373	**C1**		-0.282	1.067
O2	-0.562	-0.383	**C2**		-0.517	0.053
O3		-0.365	**C3**		0.277	0.753
H1	0.310		**C4**		0.242	0.866
H2	0.203		**C5**		-0.364	1.044
H3	0.212		**C6**		-0.484	
N2		-0.493	**C7**		0.296	
N3		-0.485	**C8**		-0.323	
N4		-0.476	H1		0.342	
O3		-0.365	H2		0.182	
			H3		0.217	
			N2			-0.926
			N3			-0.972
			N4			-0.950

Table S5. Electronic properties of the DA, UA, ZnO, [ZnO-DA and [ZnO-UA] CQDs.

	Functional: B3LYP/CEP-31g					
Compounds	E_{HF}	HOMO (eV)	LUMO (eV)	ΔE (eV)	Hardness (η, eV)	Softness (σ, eV)
Dopamine (L^1)	-516.720	-5.990	-0.416	5.574	2.787	0.359
Uric acid (L^2)	-637.767	-6.382	-1.379	5.003	2.501	0.400
ZnO wurtzite	-5487.729	-5.549	-3.271	2.278	1.139	0.878
ZnO wurtzite-Dopamine] in the corner of ZnO surface	-6003.846	-5.657	-2.976	2.681	1.341	0.746
wurtzite- uric acid at the lateral plane of ZnO surface	-6125.618	-5.631	-3.196	2.435	1.217	0.821

Table S6. TD-DFT spectral data of electronic transitions of ZnO with DA and UA at the plane with oscillator strength f > 0.0001.

Wavelength (nm)	**Osc. Strength (f)**	**ZnO wurtzite**	**Character**	**Theory (nm)**
547.3	0.1825	HOMO->LUMO (103%)	MLCT	704
546.0	0.1842	HOMO->LUMO+1 (102%)	MLCT	
284.3	0.0033	HOMO-2->LUMO (45%) HOMO-3->LUMO+1 (47%) HOMO-3->LUMO+2 (3%) HOMO-2->LUMO+3 (3%)	ILCT	283
252.5	0.0001	HOMO-4->LUMO+1 (52%) HOMO-5->LUMO (46%)	ILCT	263
247.3	0.0331	HOMO->LUMO+2 (60%) HOMO-4->LUMO (15%) HOMO-5->LUMO+1 (13%) HOMO-6->LUMO+1 (9%)	ILCT	
246.4	0.0292	HOMO->LUMO+3 (46%) HOMO-5->LUMO (22%) HOMO-4->LUMO+1 (16%) HOMO-6->LUMO (13%)	ILCT	
239.3	0.0067	HOMO-6->LUMO+1 (44%) HOMO-4->LUMO (11%) HOMO->LUMO+2 (33%) HOMO-5->LUMO+1 (9%)	ILCT	
238.9	0.015	HOMO->LUMO+3 (46%) HOMO-6->LUMO (38%) HOMO-5->LUMO (7%) HOMO-4->LUMO+1 (7%)	ILCT	
226.6	0.1579	HOMO-6->LUMO+1 (41%) HOMO-5->LUMO+1 (23%) HOMO-4->LUMO (23%)	ILCT	232

		HOMO->LUMO+2 (5%) HOMO->LUMO+1 (4%) HOMO-6->LUMO (3%)		
226.3	0.1513	HOMO-6->LUMO (42%) HOMO-5->LUMO (22%) HOMO-4->LUMO+1 (21%) HOMO->LUMO+3 (6%) HOMO->LUMO (4%) HOMO-6->LUMO+1 (3%)	ILCT	
206.7	0.0001	HOMO-5->LUMO+1 (46%) HOMO-4->LUMO (43%) HOMO->LUMO+5 (6%)	ILCT	
178.1	0.0266	HOMO-2->LUMO+3 (35%) HOMO->LUMO+4 (33%) HOMO-3->LUMO+2 (27%)	ILCT	
164.1	0.2571	HOMO->LUMO+4 (60%) HOMO-2->LUMO+3 (12%) HOMO-3->LUMO+2 (11%) HOMO-1->LUMO+5 (9%)	ILCT	
146.3	0.0288	HOMO-6->LUMO+2 (42%) HOMO-5->LUMO+2 (26%) HOMO-4->LUMO+3 (21%) HOMO-3->LUMO+4 (6%)	ILCT	
145.9	0.0313	HOMO-6->LUMO+3 (37%) HOMO-5->LUMO+3 (26%) HOMO-4->LUMO+2 (21%) HOMO-7->LUMO+1 (2%) HOMO-2->LUMO+4 (8%)	ILCT	
142.9	0.0023	HOMO-7->LUMO+1 (51%) HOMO-6->LUMO+3 (18%) HOMO-9->LUMO (7%) HOMO-8->LUMO+1 (6%) HOMO-20->LUMO (5%) HOMO-19->LUMO+1 (4%)	ILCT	
		ZnO wurtzite-Dopamine] at the parallel plane of ZnO surface		
1433.5	0.0096	HOMO->LUMO (89%) HOMO->LUMO (8%) HOMO-1->LUMO (2%)	MLCT	1421
854.9	0.0184	HOMO->LUMO (44%) HOMO-1->LUMO (35%) HOMO->LUMO+1 (10%) HOMO->LUMO (7%) HOMO-2->LUMO (4%)	MLCT	859
535.1	0.0843	HOMO->LUMO+1 (51%) HOMO->LUMO (22%) HOMO-2->LUMO (14%) HOMO-1->LUMO (5%) HOMO->LUMO (2%)	MLCT	534

		HOMO-2->LUMO+1 (2%) HOMO-1->LUMO (2%)		
529.0	0.0109	HOMO-3->LUMO (41%) HOMO-2->LUMO (26%) HOMO-2->LUMO+1 (15%) HOMO-1->LUMO (7%) HOMO->LUMO (4%) HOMO-1->LUMO (3%)	MLCT	
464.4	0.0769	HOMO-1->LUMO (42%) HOMO-2->LUMO (15%) HOMO-2->LUMO (12%) HOMO->LUMO+1 (12%) HOMO-3->LUMO (6%) HOMO-2->LUMO+1 (5%) HOMO-1->LUMO (4%) HOMO->LUMO (2%)	MLCT	464
457.4	0.0003	HOMO-2->LUMO (59%) HOMO-1->LUMO (20%) HOMO-1->LUMO (11%) HOMO-2->LUMO+1 (3%) HOMO-5->LUMO (2%) HOMO-3->LUMO (2%)	MLCT	
451.5	0.0448	HOMO-2->LUMO (32%) HOMO-1->LUMO (27%) HOMO-2->LUMO+1 (16%) HOMO-1->LUMO (8%) HOMO->LUMO (7%) HOMO-3->LUMO (5%) HOMO-1->LUMO+1 (3%)	MLCT	
442.4	0.0487	HOMO-1->LUMO (25%) HOMO-2->LUMO (20%) HOMO->LUMO+1 (21%) HOMO->LUMO (10%) HOMO-2->LUMO (8%) HOMO-2->LUMO+1 (6%) HOMO-1->LUMO (4%) HOMO-1->LUMO+1 (3%)	MLCT	
413.8	0.0181	HOMO-1->LUMO+1 (84%) HOMO-3->LUMO (4%) HOMO-4->LUMO (4%) HOMO-4->LUMO+1 (2%) HOMO-2->LUMO+1 (2%)	MLCT	
410.9	0.0123	HOMO-4->LUMO (53%) HOMO-5->LUMO (32%) HOMO-1->LUMO+1 (4%) HOMO-3->LUMO (3%) HOMO-5->LUMO (2%)	MLCT	409
399.4	0.0984	HOMO-2->LUMO+1 (40%) HOMO-3->LUMO (27%) HOMO-4->LUMO (16%) HOMO-5->LUMO(A) (8%)	MLCT	

		HOMO->LUMO (2%) HOMO->LUMO+1 (2%)		
390.4	0.051	HOMO-5->LUMO (45%) HOMO-4->LUMO (19%) HOMO-4->LUMO+1 (10%) HOMO-3->LUMO (9%) HOMO-2->LUMO+1 (9%) HOMO->LUMO (2%)	MLCT	
361.8	0.0055	HOMO-4->LUMO+1 (84%) HOMO-5->LUMO (8%) HOMO-4->LUMO (3%)	MLCT	
306.9	0.0031	HOMO-5->LUMO (64%) HOMO-6->LUMO (22%) HOMO-5->LUMO+1 (10%)	MLCT	
299.3	0.0041	HOMO->LUMO+2 (98%)	ILCT	
298.5	0.0035	HOMO-6->LUMO+1 (68%) HOMO-6->LUMO (19%) HOMO-7->LUMO (9%)	ILCT	
280.2	0.0026	HOMO-4->LUMO+1 (28%) HOMO-3->LUMO+2 (28%) HOMO-1->LUMO+3 (15%) HOMO-2->LUMO+2 (13%) HOMO-7->LUMO (4%) HOMO-6->LUMO (3%) HOMO-6->LUMO+1 (3%) HOMO-1->LUMO+2 (2%)	ILCT	
280.1	0.0191	HOMO-7->LUMO (33%) HOMO-6->LUMO+1 (25%) HOMO-6->LUMO (24%) HOMO-4->LUMO+1 (4%) HOMO-3->LUMO+2 (4%) HOMO-2->LUMO+2 (2%) HOMO-8->LUMO+1 (2%) HOMO-1->LUMO+3 (2%)	ILCT	
272.4	0.0193	HOMO->LUMO+3 (47%) HOMO->LUMO+4 (28%) HOMO->LUMO+5 (10%) HOMO->LUMO+5 (6%) HOMO-1->LUMO+3 (2%)	ILCT	
264.9	0.073	HOMO->LUMO+5 (75%) HOMO->LUMO+3 (11%) HOMO->LUMO+6 (4%) HOMO-1->LUMO+5 (2%)	ILCT	263
260.4	0.0021	HOMO->LUMO+2 (97%)	ILCT	
255.6	0.0583	HOMO-1->LUMO+2 (39%) HOMO-2->LUMO+1 (29%) HOMO-1->LUMO+1 (10%) HOMO-4->LUMO+2 (8%) HOMO-3->LUMO+3 (8%) HOMO->LUMO+2 (2%)	ILCT	

242.1	0.0187	HOMO->LUMO+3 (21%) HOMO->LUMO+4 (15%) HOMO->LUMO+6 (14%) HOMO-8->LUMO (14%), HOMO->LUMO+5 (11%) HOMO-9->LUMO (5%) HOMO-1->LUMO+3 (4%) HOMO-11->LUMO (2%), HOMO-8->LUMO+1 (2%)	ILCT	
240.9	0.0372	HOMO->LUMO+6 (29%) HOMO->LUMO+4 (16%) HOMO-8->LUMO (15%) HOMO->LUMO+5 (14%) HOMO-1->LUMO+3 (3%) HOMO->LUMO+6 (3%) HOMO-9->LUMO (2%) HOMO-1->LUMO+4 (2%) HOMO-1->LUMO+5 (2%)	ILCT	243
		ZnO wurtzite- uric acid at the corner plane of ZnO surface		
629.9	0.0026	HOMO->LUMO (98%)	MLCT	657
470.2	0.18	HOMO-1->LUMO (97%) HOMO-12->LUMO (2%)	MLCT	476
405.9	0.0063	HOMO-2->LUMO (92%) HOMO-3->LUMO (6%)	MLCT	
326.7	0.0006	HOMO-3->LUMO (94%) HOMO-2->LUMO (6%)	MLCT	
309.8	0.0932	HOMO->LUMO+1 (86%) HOMO-4->LUMO (7%) HOMO-1->LUMO+1 (4%)	MLCT	314
298.4	0.0185	HOMO-1->LUMO+1 (95%) HOMO->LUMO+1 (4%)	MLCT	
276.9	0.0014	HOMO-5->LUMO (81%) HOMO-9->LUMO (11%) HOMO-10->LUMO (2%) HOMO-8->LUMO (2%)	ILCT	
257.9	0.0108	HOMO->LUMO+3 (41%) HOMO-7->LUMO (37%) HOMO-10->LUMO (6%) HOMO-8->LUMO (7%) HOMO-5->LUMO (5%)	ILCT	
255.8	0.0247	HOMO-7->LUMO (48%) HOMO->LUMO+3 (26%) HOMO-6->LUMO (12%) HOMO-8->LUMO (6%) HOMO->LUMO+2 (6%)	ILCT	
255.08	0.0164	HOMO->LUMO+3 (26%) HOMO-8->LUMO (22%) HOMO-6->LUMO (19%)	ILCT	255

		HOMO-10->LUMO (13%) HOMO-9->LUMO (8%) HOMO-5->LUMO (7%)		
253.8	0.1368	HOMO->LUMO+2 (84%) HOMO-6->LUMO (6%) HOMO->LUMO+3 (2%)	ILCT	
252.4	0.0097	HOMO-6->LUMO (61%) HOMO-9->LUMO (8%) HOMO-7->LUMO (8%) HOMO-8->LUMO (7%) HOMO-10->LUMO (5%) HOMO->LUMO+2 (5%) HOMO-5->LUMO (2%)	ILCT	
249.4	0.0136	HOMO-8->LUMO (48%) HOMO-9->LUMO (30%) HOMO-11->LUMO (6%) HOMO-10->LUMO (6%) HOMO-6->LUMO (2%) HOMO-5->LUMO (2%)	ILCT	
236.9	0.0335	HOMO-11->LUMO (28%) HOMO-1->LUMO+3 (27%) HOMO-10->LUMO (20%) HOMO-1->LUMO+2 (15%) HOMO-8->LUMO (5%) HOMO-7->LUMO (2%)	ILCT	
236.8	0.005	HOMO-1->LUMO+2 (84%) HOMO-11->LUMO (5%) HOMO-10->LUMO (5%) HOMO-1->LUMO+3 (4%)	ILCT	
236.8	0.0096	HOMO-10->LUMO (37%) HOMO-9->LUMO (35%) HOMO-11->LUMO (14%) HOMO-1->LUMO+3 (10%)	ILCT	
230.2	0.2987	HOMO-1->LUMO+3 (51%) HOMO-11->LUMO (34%) HOMO-12->LUMO (7%)	ILCT	232
217.8	0.0338	HOMO->LUMO+4 (73%) HOMO-1->LUMO+4 (15%) HOMO->LUMO+5 (5%) HOMO->LUMO+6 (5%)	ILCT	222
217.6	0.0056	HOMO->LUMO+5 (53%) HOMO->LUMO+6 (33%) HOMO->LUMO+4 (8%)	ILCT	
215.1	0.1305	HOMO-12->LUMO (84%) HOMO-11->LUMO (8%) HOMO-1->LUMO+5 (2%)	ILCT	
187.5	0.1045	HOMO->LUMO+7 (30%) HOMO-3->LUMO+3 (23%) HOMO-6->LUMO+1 (20%) HOMO-13->LUMO (7%)	ILCT	

		HOMO-7->LUMO+1 (7%) HOMO-14->LUMO (5%) HOMO->LUMO+8 (3%)		

Table S7. TD-DFT spectra of [ZnO-DA] and [ZnO-UA] calculated at B3LYP functional with basis set: DGDZVP at gaseous state.

	λ1	λ2	λ3	λ4	λ5	λ6	λ7
ZnO wurtzite	232	263	283	704			
ZnO wurtzite-Dopamine	243	263	409	464	534	859	1421
ZnO wurtzite- uric acid	222	232	255	314	476	657	

Table S8. Electrochemical data resulted with respective to SHE for the electrodes

	CPE/CQDs (8:2)	**CPE/ZnO NPs (8:2)**
E_{pa}	0.39	0.44
E_{pc}	0.14	0.08
ΔE_p	0.25	0.36
$E_{1/2}$	0.125	0.18
R_{CT} (Ω)	184	341
Γ (nM cm^2)	5.55	2.23
k_{app} (cm/s)	4.10 x 10^{-3}	2.21 x 10^{-3}
Area (cm^2)	1.33 x 10^{-1}	5.66 x 10^{-2}

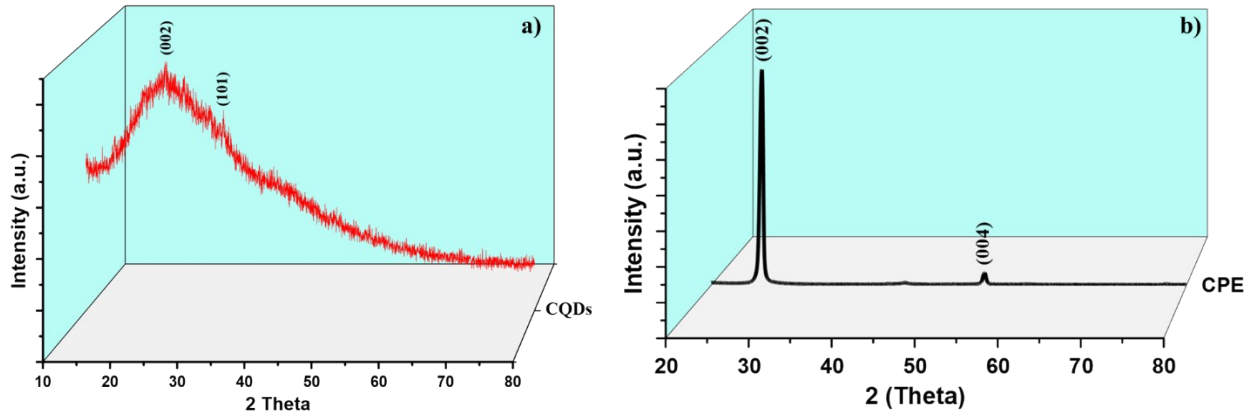

Fig. S1. XRD pattern: **a)** CQDs and **b)** CPE

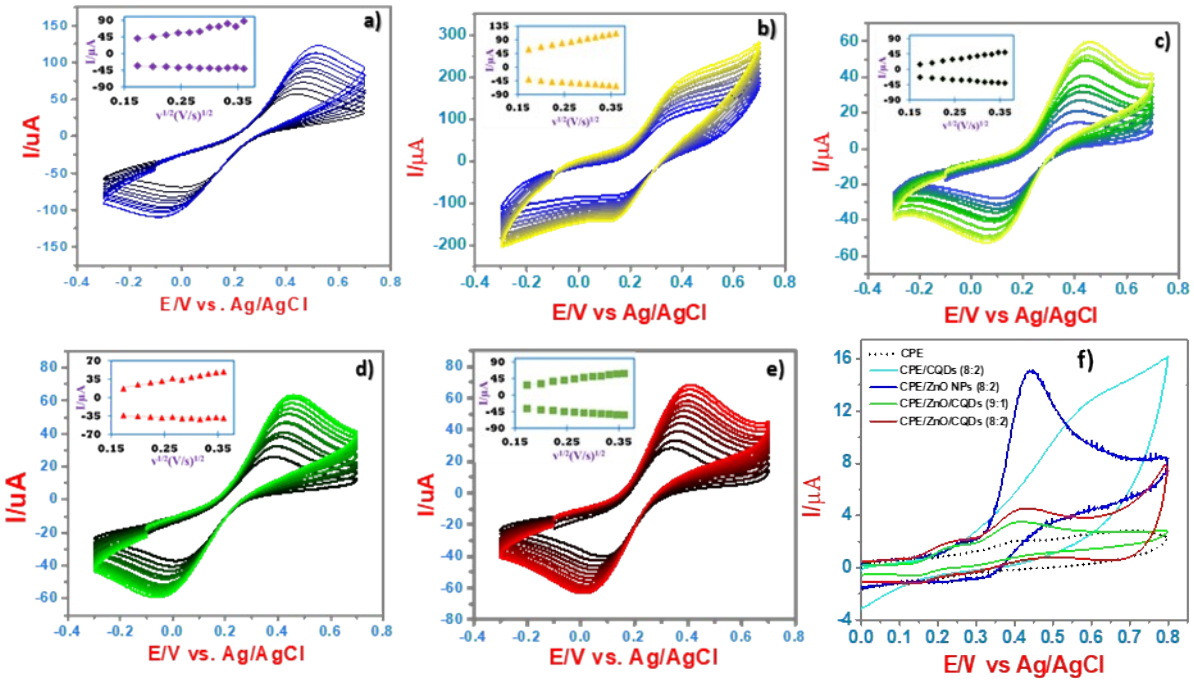

Fig. S2. a) CPE: CV at different scan rates (ν); **b)** CPE/CQDs (8:2): CV at different scan rates (ν): **c)** CPE/ZnO NPs (8:2): CV at different scan rates (ν); **d)** CPE/ZnO/CQDs (9:1): CV at different scan rates (ν); **e)** CPE/ZnO/CQDs (8:2): CV at different scan rates (ν); f) CV for DA(50 µM) and UA (500 µM) using CPE, CPE/CQDs (8:2), CPE/ZnO NPs (8:2), CPE/ZnO/CQDs (9:1), and CPE/ZnO/CQDs (8:2): B-R buffer (pH 7.0, 0.04 M); scan rate: 50 mV/s

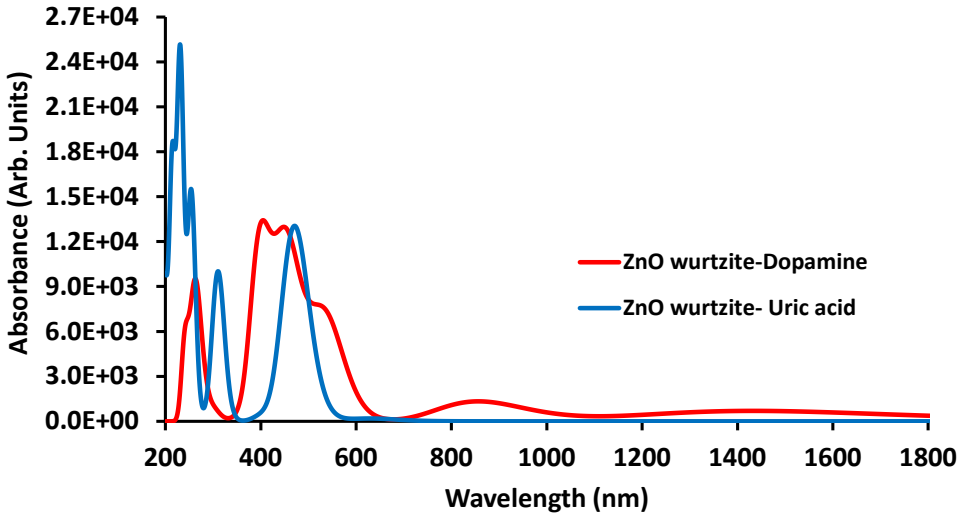

Figure. S3. TD-DFT spectra of with dopamine (DA), uric acid (UA), [ZnO-DA] at the parallel plane surface to ZnO and [ZnO-UA] in the corner position with ZnO at b3lyp/dgdzvp basis set at gaseous state.

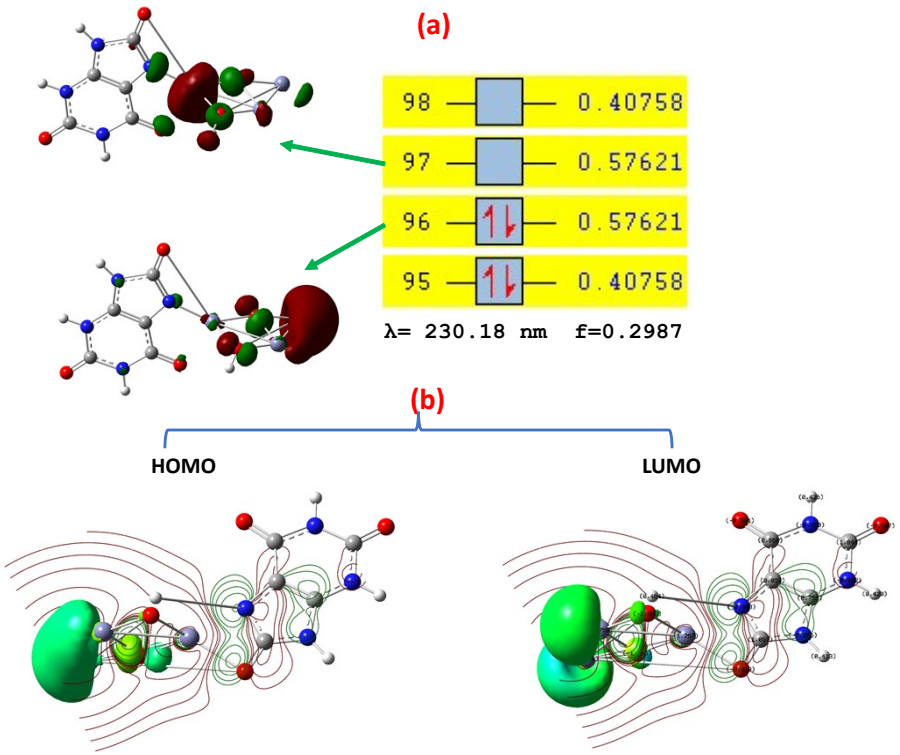

Figure. S4 (a) NTOs at B3LYP/DGDZVP basis set, orbital 96 (particle), and orbital 97 (hole) for [ZnO–UA], excited state number 19 at S = 0. (b) Electron density isosurface for [ZnO–UA] at gaseous state: the code of color for the structure C (grey), H (white), N (blue), O (red) and Zn (gray/lavender), and (contour 0.05 e Å−3), HOMO and LUMO determined by B3LYP/DGDZVP: HOMO and LUMO contour plots (isosurface value = 0.05 au).

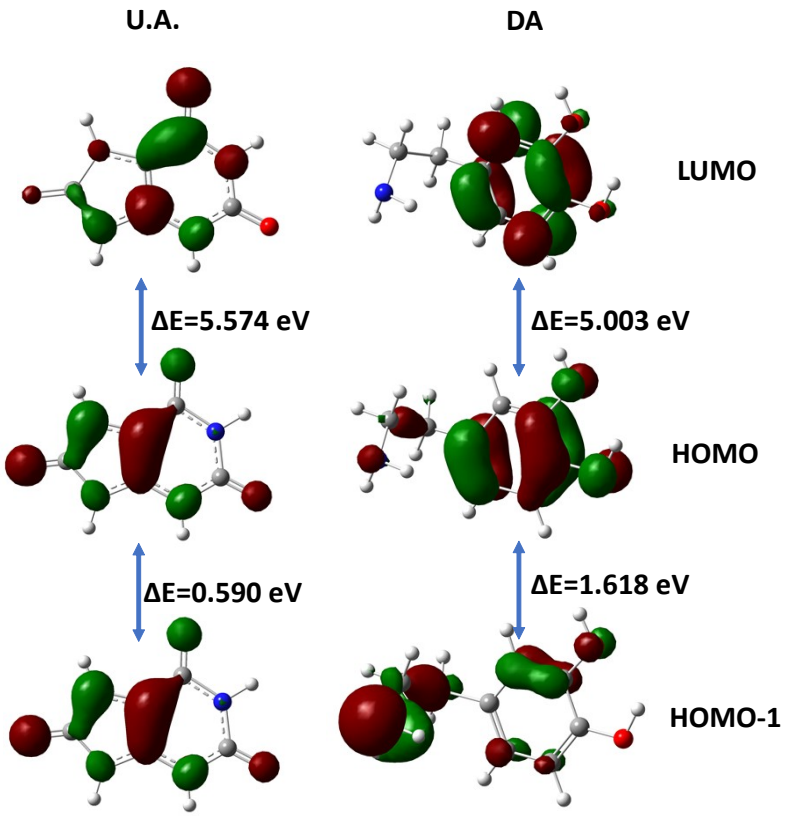

Figure. S5. Molecular orbital HOMO-LUMO of a) **DA** and b) **UA** at gaseous state.

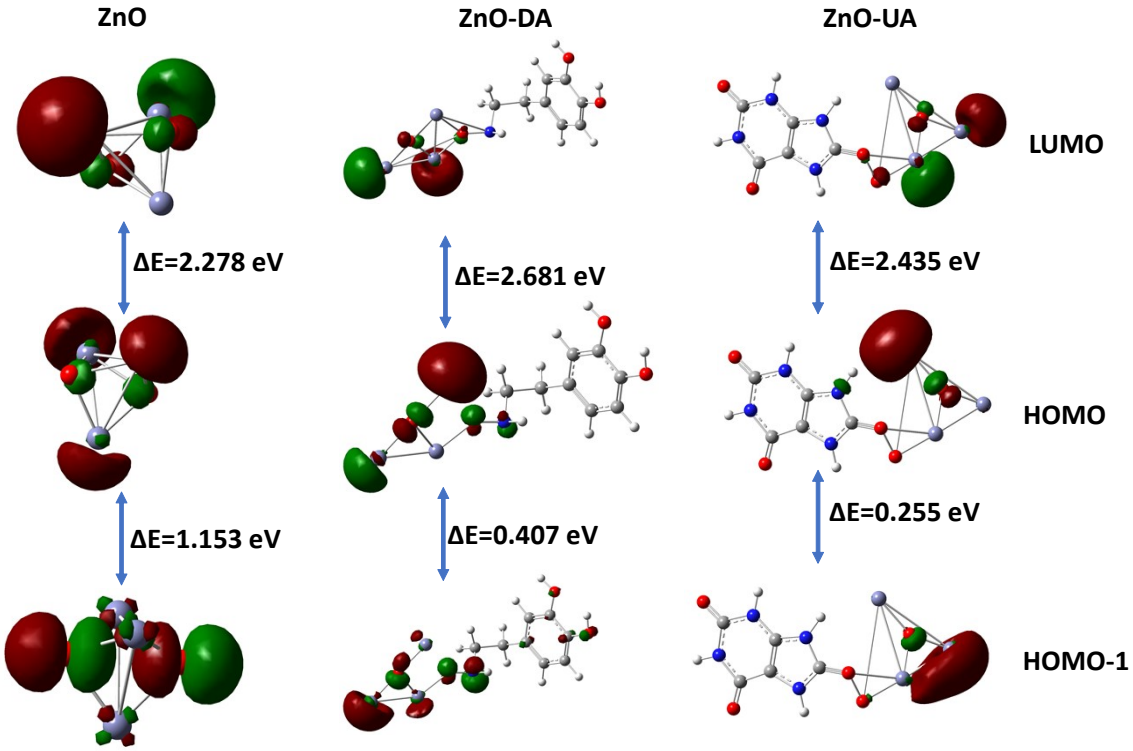

Fig. S6. Molecular orbital HOMO-LUMO of a) **ZnO-DA** and b) **ZnO-UA** at gaseous state.

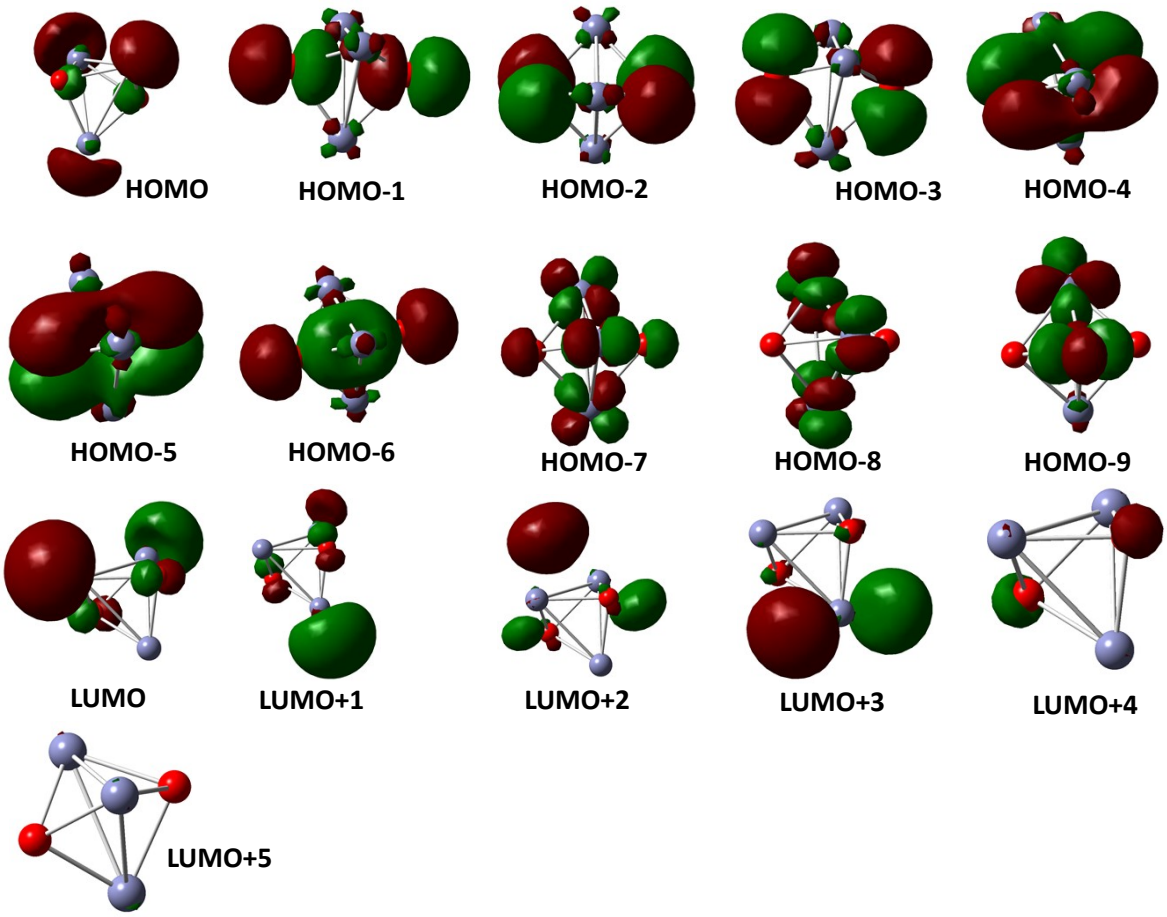

Figure. S7. Frontier molecular orbitals of ZnO (HOMOs and LUMOs) analysis:

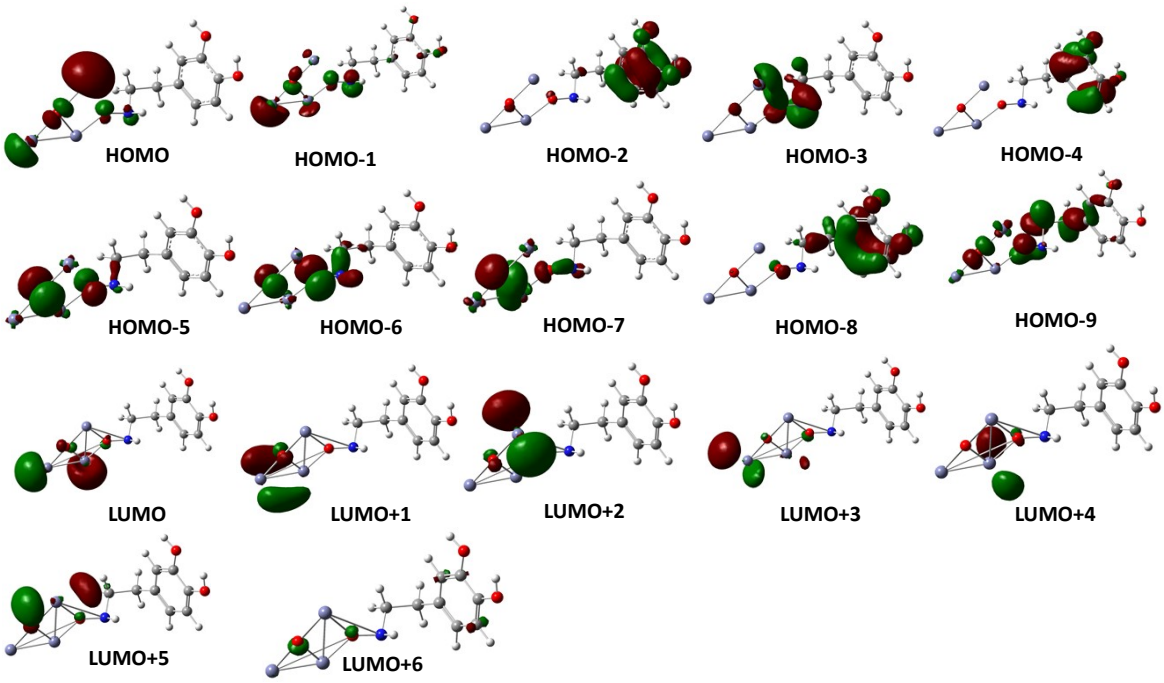

Figure. S8. Frontier molecular orbitals of [ZnO-DA] (HOMOs and LUMOs) analysis.

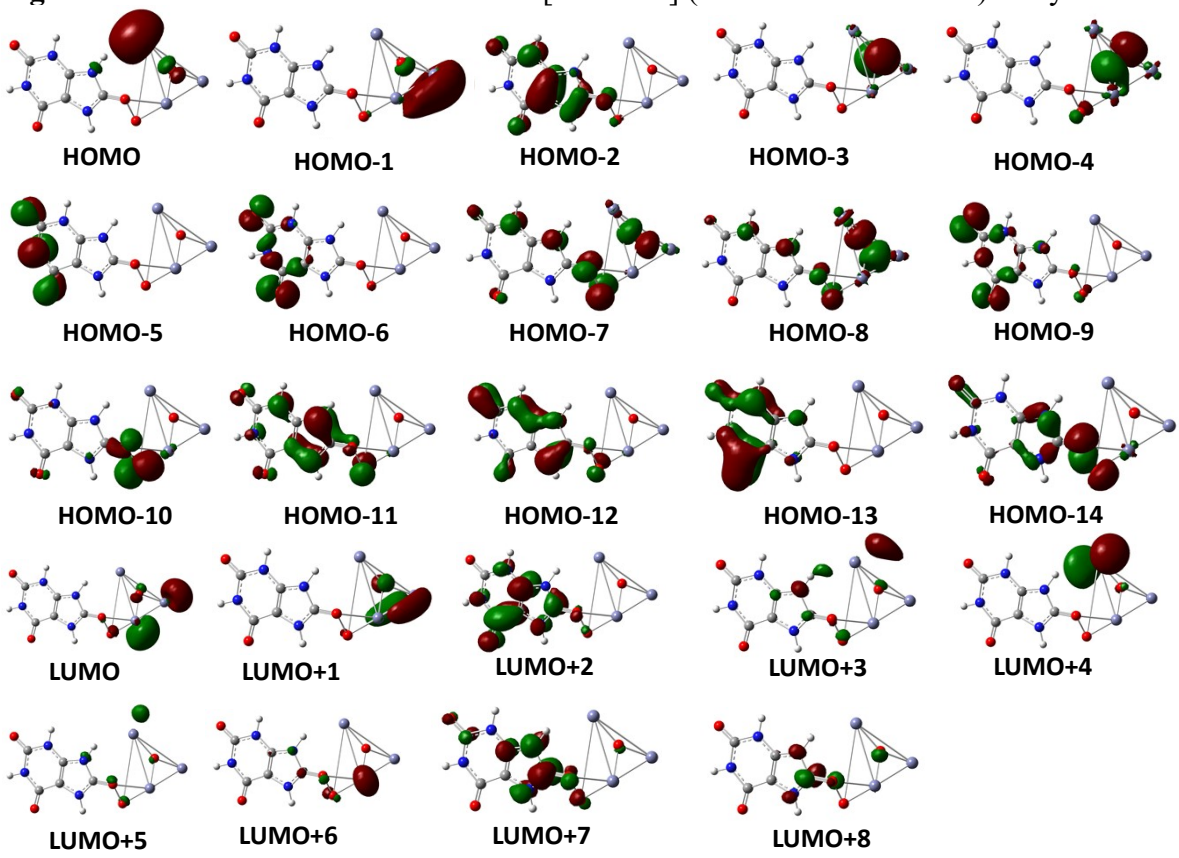

Figure. S9. Frontier molecular orbitals of [ZnO-UA] (HOMOs and LUMOs) analysis.

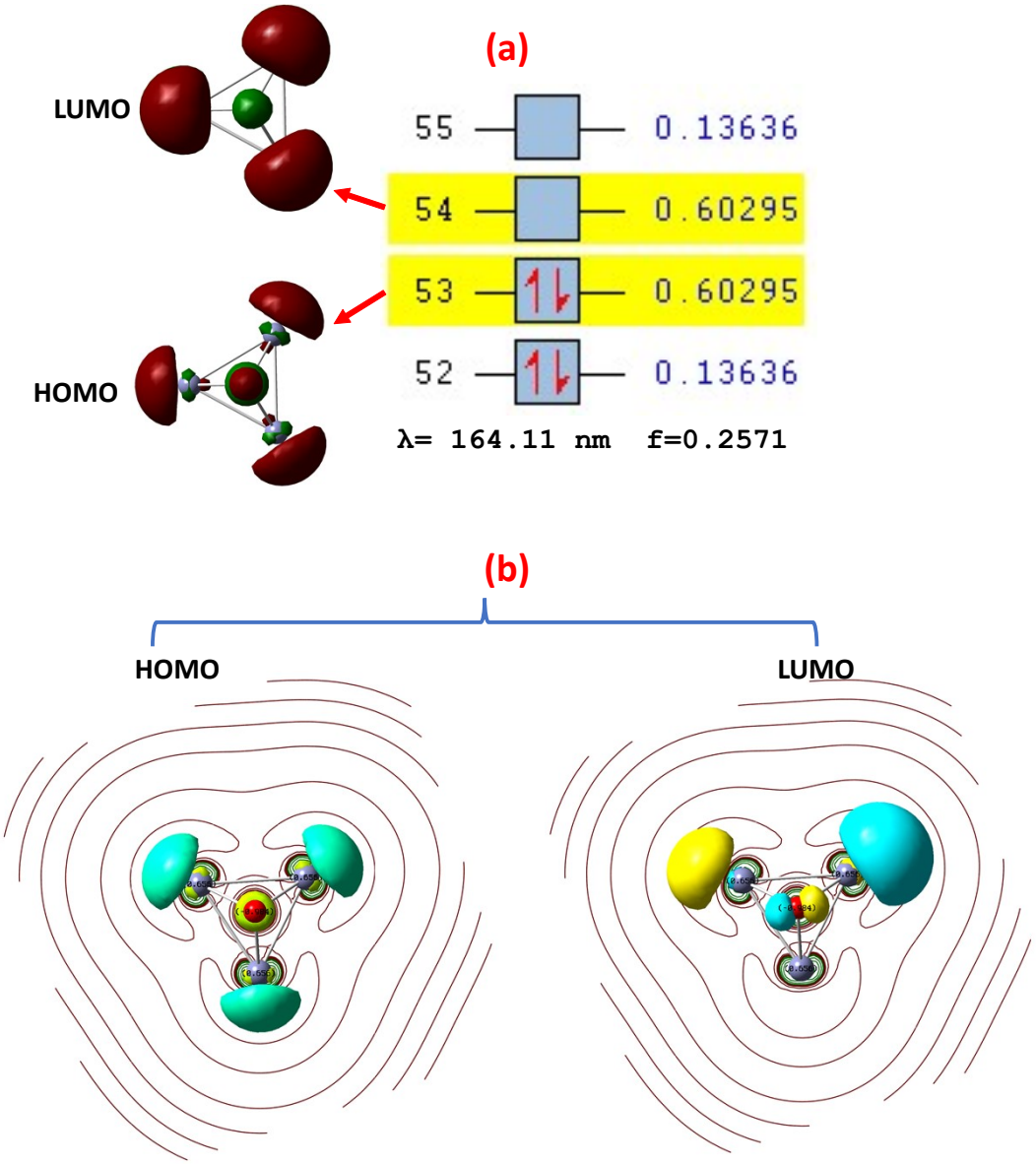

Figure. S10 (a) NTOs at B3LYP/DGDZVP basis set, orbital 53 (particle), and orbital 54 (hole) for [ZnO], excited state number 23 at S = 0. (b) Electron density isosurface for [ZnO] at gaseous state: the code of color for the structure C (grey), H (white), N (blue), O (red) and Zn (gray/lavender), and (contour 0.05 e Å−3), HOMO and LUMO determined by B3LYP/DGDZVP: HOMO and LUMO contour plots (isosurface value = 0.05 au).