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Supporting Information

An Efficient Heterodinuclear Ir(III)/Pt(II) Complex: Synthesis, Photophysics and Application in Light-Emitting Electrochemical Cells

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Table S1. Crystallographic data for complex **2.**

Formula	$C_{58}H_{67}IrN_4O_4Pt$
$D_{calc.}$/ g cm^{-3}	1.452
μ/mm^{-1}	9.146
Formula Weight	1271.44
Colour	clear red
Shape	needle
Size/mm^3	0.34×0.09×0.05
T/K	123.01(10)
Crystal System	orthorhombic
Flack Parameter	0.003(8)
Hooft Parameter	0.001(3)
Space Group	$Pca2_1$
a/Å	17.6736(2)
b/Å	20.2100(2)
c/Å	16.28070(10)
α/°	90
β/°	90
γ/°	90
V/Å^3	5815.20(9)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	CuK_α
Θ_{min}/°	3.322
Θ_{max}/°	76.635
Measured Refl.	69489
Independent Refl.	11699
Reflections with I > 2(I)	11482
R_{int}	0.0387
Parameters	685
Restraints	109
Largest Peak	1.244
Deepest Hole	-0.681
GooF	1.021
wR_2 (all data)	0.0707
wR_2	0.0700
R_1 (all data)	0.0276
R_1	0.0270

Table S2. The bond lengths and bond angles derived from XRD measurements on complex **2** and from DFT calculations on complex **2'** in the S_0 ground state and in the T_1 emissive state. The atom numbering is presented in Figure 1(a).

Bond	XRD (esd)	DFT: S_0	DFT: T_1
Bond length (Å)			
Pt-C1	1.966(6)	1.978	1.982
Pt-N1	1.996(4)	2.030	2.017
Pt-O1	2.010(4)	2.035	2.049
Pt-O2	2.094(5)	2.150	2.177
Ir-C7	1.997(6)	1.994	1.970
Ir-C8	1.995(5)	1.997	1.991
Ir-N2	2.042(5)	2.068	2.056

Ir-N3	2.038(5)	2.055	2.071
Ir-O3	2.145(4)	2.190	2.179
Ir-O4	2.158(4)	2.186	2.171
Bond angle (°)			
C1-Pt-N1	81.0(2)	80.854	81.129
C1-Pt-O1	93.4(3)	93.639	94.003
C1-Pt-O2	175.0(2)	175.896	175.891
N1-Pt-O1	173.3(2)	174.492	175.095
O1-Pt-O2	91.6(2)	90.449	89.661
C7-Ir-N2	80.2(2)	80.379	82.193
C7-Ir-N3	94.7(2)	97.657	96.973
C7-Ir-O4	175.1(2)	175.945	172.460
C7-Ir-O3	87.9(2)	91.969	91.064
C7-Ir-C8	92.2(2)	89.939	94.612
N2-Ir-C8	93.8(2)	98.366	98.130
N2-Ir-N3	172.11(18)	177.618	178.400
N2-Ir-O3	89.14(16)	85.399	86.636
N2-Ir-O4	96.42(16)	95.795	92.544
C8-Ir-N3	80.3(2)	80.238	80.560
C8-Ir-O3	177.0(2)	176.021	173.028
C8-Ir-O4	91.64(19)	91.960	91.465
O3-Ir-O4	88.44(16)	86.358	83.209
Torsion angle (°)			
O1-Pt-C1-C2	172.8(4)	179.802	177.202
O2-Pt-N1-C3	176.9(4)	179.472	175.204
C6-C7-Ir-C8	98.9(5)	101.788	103.586
C5-N2-Ir-N3	52.3(15)	38.466	65.518
C6-C7-Ir-O3	84.0(4)	81.704	80.465
C5-N2-Ir-O4	173.7(4)	174.704	167.711
N2-Ir-O3-C14	102.6(5)	94.023	72.811
N2-Ir-O4-C15	99.5(5)	86.713	63.604

Table S3. DFT optimized geometries of complex **2'** in cartesian (XYZ) coordinates.

Ground state (S_0)				Lowest triplet state (T_1)			
C	4.040186000	-0.075141000	0.990373000	C	4.028891000	-0.437140000	0.891470000
N	3.446032000	-0.004150000	-0.234372000	N	3.504849000	0.055580000	-0.263149000
C	5.391473000	-0.414527000	1.059052000	C	5.371491000	-0.802771000	0.918600000
C	6.086918000	-0.669441000	-0.124355000	C	6.135496000	-0.648432000	-0.243227000
N	5.456471000	-0.586391000	-1.314102000	N	5.574134000	-0.146396000	-1.361297000
C	4.184861000	-0.263698000	-1.319389000	C	4.303589000	0.178495000	-1.328953000
C	7.516285000	-1.035837000	-0.147626000	C	7.562675000	-1.008943000	-0.311190000
C	8.288035000	-1.124124000	1.020072000	C	8.236664000	-1.607095000	0.763877000
C	9.630647000	-1.474579000	0.961206000	C	9.581996000	-1.935427000	0.665157000
C	10.256422000	-1.748652000	-0.261151000	C	10.307787000	-1.678008000	-0.504709000
C	9.482563000	-1.663882000	-1.424969000	C	9.630698000	-1.086318000	-1.578356000
C	8.140552000	-1.312894000	-1.372679000	C	8.285628000	-0.757510000	-1.486886000
C	3.157690000	0.236854000	2.097473000	C	3.082034000	-0.503310000	1.994014000
C	1.823128000	0.556967000	1.733658000	C	1.768715000	-0.044878000	1.706432000
C	0.936907000	0.898858000	2.764553000	C	0.813220000	-0.065985000	2.729315000
C	1.328089000	0.912574000	4.105790000	C	1.125030000	-0.526498000	4.011432000
C	2.655354000	0.578213000	4.434653000	C	2.430748000	-0.983498000	4.266292000
C	3.560734000	0.246576000	3.442481000	C	3.400009000	-0.971027000	3.274270000
C	0.364443000	1.275865000	5.191367000	C	0.105130000	-0.526863000	5.104858000
C	11.709925000	-2.095895000	-0.323322000	C	11.764286000	-2.003441000	-0.595686000
H	5.877902000	-0.477432000	2.033389000	H	5.804023000	-1.193936000	1.840241000
H	3.658274000	-0.187099000	-2.280137000	H	3.831407000	0.590680000	-2.230690000
H	7.844350000	-0.919098000	1.997972000	H	7.711389000	-1.834465000	1.695232000
H	10.211698000	-1.540285000	1.887212000	H	10.085278000	-2.408100000	1.515089000
H	9.946996000	-1.881528000	-2.392871000	H	10.174638000	-0.883217000	-2.507006000
H	7.543485000	-1.249670000	-2.285349000	H	7.764779000	-0.298435000	-2.330293000
H	-0.100399000	1.165945000	2.524703000	H	-0.204068000	0.291233000	2.531227000
H	2.967667000	0.586450000	5.484401000	H	2.680995000	-1.354292000	5.265777000
H	4.590977000	-0.006182000	3.715076000	H	4.408174000	-1.331529000	3.501722000
H	0.248640000	0.449611000	5.912889000	H	0.094374000	-1.489048000	5.641622000
H	0.723009000	2.145476000	5.767420000	H	0.331886000	0.250339000	5.854545000
H	-0.631098000	1.519355000	4.792292000	H	-0.906565000	-0.333698000	4.720063000
H	11.934106000	-2.751778000	-1.178337000	H	12.064971000	-2.233767000	-1.628994000
H	12.327509000	-1.188765000	-0.443572000	H	12.379368000	-1.148595000	-0.264670000
H	12.048699000	-2.595430000	0.597062000	H	12.031093000	-2.858107000	0.044270000
Ir	1.437245000	0.430514000	-0.222044000	Ir	1.483071000	0.500249000	-0.187471000
C	-0.826528000	2.275801000	-0.341444000	C	-0.767435000	2.342301000	0.049416000
N	-0.566091000	0.940362000	-0.167035000	N	-0.516740000	0.961337000	-0.058890000
C	-2.153066000	2.700208000	-0.393902000	C	-2.099141000	2.767633000	0.034181000
C	-3.176808000	1.768650000	-0.274426000	C	-3.130249000	1.848592000	-0.049296000
N	-2.852400000	0.445274000	-0.098202000	N	-2.804741000	0.475918000	-0.073619000
C	-1.574549000	0.087466000	-0.052897000	C	-1.531491000	0.117669000	-0.085472000
C	-4.600335000	2.021220000	-0.318961000	C	-4.549927000	2.092170000	-0.099862000
C	-5.178505000	3.289643000	-0.488170000	C	-5.148839000	3.363316000	-0.111925000
C	-6.555882000	3.419448000	-0.520950000	C	-6.529354000	3.484424000	-0.161366000
C	-7.387310000	2.291003000	-0.386639000	C	-7.353243000	2.346529000	-0.202767000
C	-6.803426000	1.032434000	-0.217512000	C	-6.751859000	1.081495000	-0.184969000
C	-5.415442000	0.869710000	-0.180415000	C	-5.365294000	0.927055000	-0.135366000
C	0.353217000	3.103043000	-0.447430000	C	0.417073000	3.135340000	0.190498000
C	1.593243000	2.411963000	-0.378769000	C	1.675424000	2.428013000	0.171805000
C	2.763732000	3.181813000	-0.451008000	C	2.868767000	3.145498000	0.353473000
C	2.732005000	4.569636000	-0.601549000	C	2.880892000	4.527172000	0.534125000
C	1.486066000	5.223430000	-0.677495000	C	1.636735000	5.199156000	0.535566000
C	0.311242000	4.500279000	-0.599397000	C	0.433578000	4.529958000	0.374367000
C	3.992999000	5.370044000	-0.684615000	C	4.150903000	5.295284000	0.719282000
C	-8.873708000	2.456550000	-0.429816000	C	-8.841627000	2.490139000	-0.290383000

H	-2.387766000	3.756396000	-0.535828000	H	-2.331476000	3.834568000	0.091875000
H	-1.346345000	-0.976273000	0.089837000	H	-1.314460000	-0.958847000	-0.099642000
H	-4.548386000	4.179017000	-0.594195000	H	-4.527812000	4.265752000	-0.080861000
H	-7.010092000	4.407359000	-0.652210000	H	-6.988412000	4.479494000	-0.167477000
H	-7.445030000	0.150106000	-0.110614000	H	-7.385575000	0.186550000	-0.205425000
H	3.743068000	2.690032000	-0.389495000	H	3.827157000	2.611161000	0.353829000
H	1.456229000	6.311825000	-0.795069000	H	1.627277000	6.286401000	0.675398000
H	-0.648959000	5.023897000	-0.654764000	H	-0.503987000	5.094040000	0.399003000
H	4.063690000	5.898941000	-1.650170000	H	4.293271000	6.042494000	-0.080543000
H	4.024315000	6.145696000	0.098796000	H	4.152200000	5.853189000	1.671454000
H	4.887706000	4.739585000	-0.577235000	H	5.029149000	4.632609000	0.717330000
H	-9.396778000	1.502065000	-0.272866000	H	-9.358601000	1.590878000	0.078587000
H	-9.218068000	3.166680000	0.340517000	H	-9.202243000	3.356428000	0.287431000
H	-9.199365000	2.866803000	-1.400713000	H	-9.170008000	2.645873000	-1.333602000
Pt	-4.427171000	-0.826836000	0.055576000	Pt	-4.376004000	-0.789045000	-0.071962000
O	1.119131000	-1.728169000	-0.096065000	O	1.071984000	-1.548861000	-0.773616000
O	1.139833000	0.207473000	-2.380670000	O	1.300675000	0.875604000	-2.325830000
C	0.861720000	-0.866465000	-2.988949000	C	0.725858000	0.148681000	-3.190691000
C	0.911026000	-2.510921000	-1.067915000	C	0.486287000	-1.939751000	-1.829859000
C	0.756167000	-2.152316000	-2.422012000	C	0.286471000	-1.171822000	-2.990290000
O	-3.222778000	-2.588826000	0.316509000	O	-3.172239000	-2.597859000	0.067338000
C	-3.704404000	-3.743946000	0.495260000	C	-3.666483000	-3.747258000	0.248458000
C	-5.075278000	-4.074873000	0.532041000	C	-5.039664000	-4.067106000	0.282913000
C	-6.163374000	-3.206417000	0.377306000	C	-6.123648000	-3.192889000	0.112479000
O	-6.121645000	-1.946574000	0.184237000	O	-6.075301000	-1.933149000	-0.054384000
C	-2.701567000	-4.844967000	0.672449000	C	-2.683257000	-4.872931000	0.407707000
C	-7.553557000	-3.763029000	0.437046000	C	-7.515004000	-3.753151000	0.124902000
C	0.835675000	-3.965877000	-0.703193000	C	-0.075992000	-3.325285000	-1.780592000
C	0.644312000	-0.719404000	-4.468309000	C	0.526333000	0.787551000	-4.531600000
H	0.541670000	-2.969810000	-3.115598000	H	-0.210323000	-1.664412000	-3.829859000
H	-5.318222000	-5.127906000	0.694879000	H	-5.288796000	-5.120176000	0.439317000
H	-2.001641000	-4.573035000	1.478566000	H	-1.805870000	-4.525142000	0.973412000
H	-2.104246000	-4.939279000	-0.249036000	H	-2.326271000	-5.190300000	-0.587272000
H	-3.160366000	-5.815872000	0.900340000	H	-3.121174000	-5.751179000	0.901835000
H	-7.574589000	-4.847346000	0.605717000	H	-7.540804000	-4.840038000	0.277048000
H	-8.078252000	-3.531640000	-0.503583000	H	-8.012027000	-3.508986000	-0.827537000
H	-8.112840000	-3.259172000	1.241355000	H	-8.098752000	-3.260481000	0.918714000
H	0.186875000	-4.086376000	0.177571000	H	-1.042978000	-3.264747000	-1.247153000
H	1.839266000	-4.310907000	-0.403894000	H	0.581638000	-3.984056000	-1.194654000
H	0.475242000	-4.602965000	-1.522557000	H	-0.258187000	-3.752193000	-2.776198000
H	1.538954000	-0.264508000	-4.923012000	H	1.494610000	1.153086000	-4.908333000
H	-0.185288000	-0.015396000	-4.641943000	H	-0.118631000	1.673177000	-4.414061000
H	0.423279000	-1.668920000	-4.973635000	H	0.078308000	0.110399000	-5.270498000

Table S4. Selected TD-DFT transitions of the model complex **2'** in the ground state (S_0) geometry.

State, energy (eV)	*f* (oscillator strength)	Contributing transition coefficients*	Character**
triplets			
T_1, 1.868	(triplet)	HOMO→LUMO (0.70)	$M^{Ir(III)}L^{dpp1}CT/L^{dpp2}L^{dpp1}CT/LC^{dpp1}$
T_2, 2.016	(triplet)	HOMO→LUMO+1 (0.70)	$M^{Ir(III)}L^{dpp2}CT/L^{dpp1}L^{dpp2}CT/LC^{dpp2}$
T_3, 2.104	(triplet)	HOMO−3→LUMO (0.16) HOMO−1→LUMO (0.68)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT/L^{dpp2}L^{dpp1}CT/LC^{dpp2}$
singlets			
S_1, 1.992	0.0706	HOMO→LUMO (0.69) HOMO−1→LUMO (0.10)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT/\ L^{acac2}L^{dpp1}CT$
S_2, 2.125	0.0138	HOMO→LUMO+1 (0.69)	$M^{Ir(III)}L^{dpp2}CT/L^{dpp1}L^{dpp2}CT/LC^{dpp2}$
S_3, 2.237	0.0624	HOMO−1→LUMO (0.10) HOMO−2→LUMO (0.67)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT/\ LC^{dpp1}/\ L^{acac1}L^{dpp1}CT$
S_4, 2.367	0.0349	HOMO−1→LUMO+1 (-0.10) HOMO−2→LUMO+1 (0.68)	$M^{Ir(III)/Pt(II)}L^{dpp2}CT/L^{acac1}L^{dpp1}CT/L^{dpp1}L^{dpp2}CT$
S_5, 2.444	0.1232	HOMO−3→LUMO (-0.21) HOMO−2→LUMO (0.64) HOMO−1→LUMO (-0.10) HOMO−2→LUMO+1 (0.14)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT/\ LC^{dpp1}/\ L^{acac1}L^{dpp1}CT$
S_6, 2.496	0.0023	HOMO−2→LUMO (-0.11) HOMO−2→LUMO+1 (0.68)	$M^{Pt(II)}L^{dpp2}CT/\ L^{dpp1}L^{dpp2}CT/\ L^{acac1}L^{dpp2}CT$
S_7, 2.535	0.0225	HOMO→LUMO+2 (0.69)	$M^{Ir(III)}L^{dpp1}CT/L^{dpp2}L^{dpp1}CT/LC^{dpp1}$
S_8, 2.593	0.0070	HOMO−4→LUMO (0.69) HOMO−3→LUMO (0.13)	$M^{Pt(II)/Ir(III)}L^{dpp1}CT/LC^{dpp1}$
S_9, 2.620	0.1125	HOMO−4→LUMO (-0.14) HOMO−3→LUMO (0.63) HOMO−3→LUMO+1 (0.13) HOMO−2→LUMO (0.21)	$M^{Ir(III)/Pt(II))}L^{dpp1}CT/LC^{dpp1}$
S_{10}, 2.665	0.0233	HOMO−5→LUMO+1 (0.13) HOMO−3→LUMO (-0.12) HOMO−3→LUMO+1 (0.60) HOMO→LUMO+3 (0.32)	$M^{Ir(III)/Pt(II)}L^{dpp2}CT$

S_{11}, 2.700	0.0748	HOMO−5→LUMO (0.65) HOMO−1→LUMO+2 (0.10) HOMO→LUMO+3 (0.20)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT$
S_{12}, 2.717	0.0070	HOMO−5→LUMO (-0.19) HOMO−5→LUMO+1 (-0.19) HOMO−3→LUMO+1 (-0.26) HOMO−1→LUMO+2 (-0.12) HOMO→LUMO+3 (0.57)	$M^{Ir(III)}L^{dpp2}CT/L^{dpp1}L^{dpp2}CT/LC^{dpp2}$
S_{13}, 2.734	0.0001	HOMO−4→LUMO+1 (0.70)	$M^{Pt(II)}L^{dpp2}CT$
S_{14}, 2.785	0.0477	HOMO−5→LUMO (-0.12) HOMO−5→LUMO+1 (-0.12) HOMO−1→LUMO+2 (0.66)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT$

*Square of the coefficient multiplied by two gives percentage contribution of the transition to formation of the excited state

**MLCT – Metal-to-Ligand Charge Transfer; LLCT – Ligand-to-Ligand Charge transfer; LC – Ligand Centered.

Table S5. Selected TD-DFT transitions of the model complex **2'** in the lowest triplet state (T_1) geometry.

State, energy (eV)	*f* (oscillator strength)	Contributing transition coefficients*	Character**
triplets			
T_1, 1.615	(triplet)	HOMO→LUMO (0.70)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT/L^{dpp2}L^{dpp1}CT/LC^{dpp1}$
T_2, 1.921	(triplet)	HOMO−1→LUMO (0.68) HOMO−3→LUMO (0.16)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT$
T_3, 1.931	(triplet)	HOMO→LUMO+1 (0.70)	$M^{Ir(III)}L^{dpp2}CT/L^{dpp1}L^{dpp2}CT/LC^{dpp2}$
singlets			
S_1, 1.805	0.1058	HOMO→LUMO (0.69) HOMO−1→LUMO (0.12)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT$
S_2, 2.028	0.0203	HOMO→LUMO+1 (0.70)	$M^{Ir(III)}L^{dpp2}CT/L^{dpp1}L^{dpp2}CT/LC^{dpp2}$
S_3, 2.088	0.0707	HOMO→LUMO (-0.11) HOMO−1→LUMO (0.68) HOMO−3→LUMO (-0.10)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT$
S_4, 2.348	0.1126	HOMO−1→LUMO+1 (-0.17) HOMO−2→LUMO (0.61) HOMO−3→LUMO (-0.30)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT$/ $M^{Ir(III)/Pt(II)}L^{dpp2}CT$

S_5, 2.360	0.0362	HOMO─1→LUMO+1 (0.66) HOMO─2→LUMO (-0.15)	$M^{Ir(III)/Pt(II)}L^{dpp2}CT$/ $M^{Ir(III)/Pt(II)}L^{dpp1}CT$
S_6, 2.476	0.0497	HOMO─4→LUMO (0.49) HOMO─3→LUMO (0.41) HOMO─2→LUMO (0.20) HOMO→LUMO+2 (-0.20)	$M^{Ir(III)}L^{dpp1}CT/L^{acac1}L^{dpp1}CT$
S_7, 2.484	0.0469	HOMO─4→LUMO (0.50) HOMO─3→LUMO (-0.40) HOMO─2→LUMO (-0.17) HOMO→LUMO+2 (0.21)	$M^{Ir(III)}L^{dpp1}CT/L^{acac1}L^{dpp1}CT$
S_8, 2.505	0.0319	HOMO─3→LUMO (0.25) HOMO─2→LUMO (0.13) HOMO→LUMO+2 (0.63)	$M^{Ir(III)}L^{dpp1}CT/L^{acac1}L^{dpp1}CT$
S_9, 2.532	0.0045	HOMO─2→LUMO+1 (0.70)	$M^{Ir(III)/Pt(II)}L^{dpp2}CT/L^{dpp1}L^{dpp2}CT$/ $L^{acac1}L^{dpp2}CT$
S_{10}, 2.575	0.0352	HOMO─5→LUMO (0.659)	$M^{Ir(III)/Pt(II)}L^{dpp1}CT$

*Square of the coefficient multiplied by two gives percentage contribution of the transition to formation of the excited state

**MLCT – Metal-to-Ligand Charge Transfer; LLCT – Ligand-to-Ligand Charge transfer; LC – Ligand Centered.

Table S6. DFT calculated frontier orbital energy levels and involved contributions of complex **2'** resulting from Mulliken population analysis in the ground state (S_0) relaxed geometry.

Orbital	Energy, (eV)	Contributions, (%)					
		Pt	Ir	dpp1[a]	dpp2[b]	acac1[c]	acac2[d]
LUMO+4	-1.71	3	0	3	0	94	0
LUMO+3	-2.07	0	1	4	95	0	0
LUMO+2	-2.23	1	1	92	4	2	0
LUMO+1	-2.66	0	5	1	94	0	1
LUMO	-2.81	4	4	89	1	2	0
HOMO	-4.74	2	47	22	21	1	6
HOMO−1	-4.99	4	39	10	5	1	41
HOMO−2	-5.14	33	8	31	2	21	6
HOMO−3	-5.29	31	22	18	7	18	4
HOMO−4	-5.39	91	0	5	0	3	0

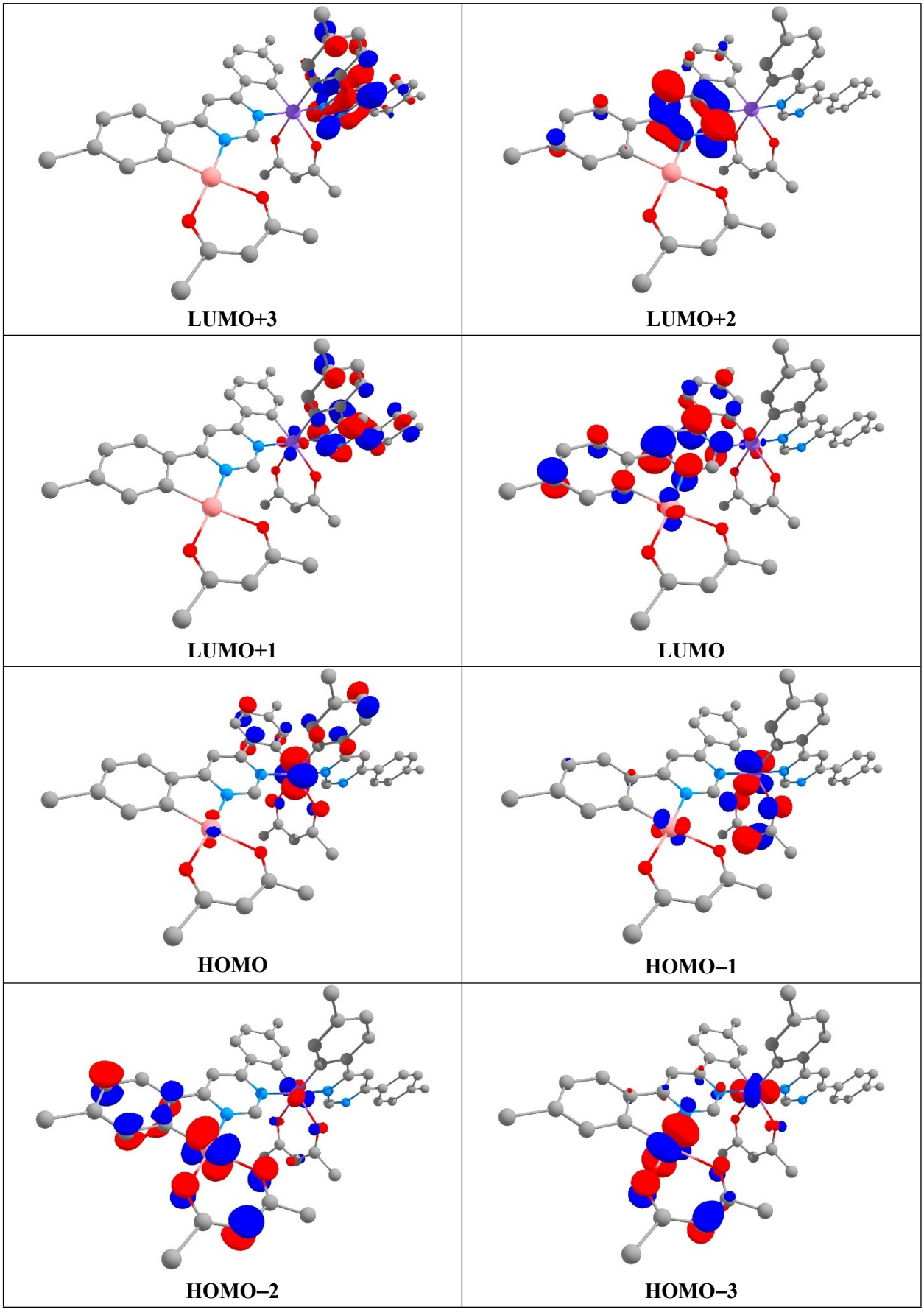
a) dpp1 – Pt(II)/Ir(III) two-coordinated diphenylpyrimidine
b) dpp2 – Ir(III) mono-coordinated diphenylpyrimidine
c) acac1 – Pt(II) coordinated acetylacetonate
d) acac2 – Ir(III) coordinated acetylacetonate

Table S7. DFT calculated frontier orbital energy levels and involved contributions of complex **2'** resulting from Mulliken population analysis in the lowest triplet state (T_1) geometry.

Orbital	Energy, (eV)	Contributions, (%)					
		Pt	Ir	dpp1[a]	dpp2[b]	acac1[c]	acac2[d]
LUMO+4	-1.70	3	0	4	0	92	2
LUMO+3	-2.05	0	1	11	87	1	0
LUMO+2	-2.17	1	1	83	12	2	1
LUMO+1	-2.65	0	4	1	94	0	1
LUMO	-2.94	5	5	89	1	1	1
HOMO	-4.63	2	42	25	20	1	10
HOMO−1	-4.96	3	40	11	7	0	39
HOMO−2	-5.18	35	4	31	1	26	3
HOMO−3	-5.30	33	20	19	6	15	7
HOMO−4	-5.41	91	0	6	0	3	0

a) dpp1 – Pt(II)/Ir(III) two-coordinated diphenylpyrimidine
b) dpp2 – Ir(III) mono-coordinated diphenylpyrimidine
c) acac1 – Pt(II) coordinated acetylacetonate
d) acac2 – Ir(III) coordinated acetylacetonate

Table S8. M06L/def2-SVP/C-PCM Iso-surface contour plots (iso-value = 0.05) of selected orbitals of model complex **2'** at the relaxed ground state (S_0) geometry (M06/def2-SVP/C-PCM).


LUMO+3
LUMO+2
LUMO+1
LUMO
HOMO
HOMO–1
HOMO–2
HOMO–3

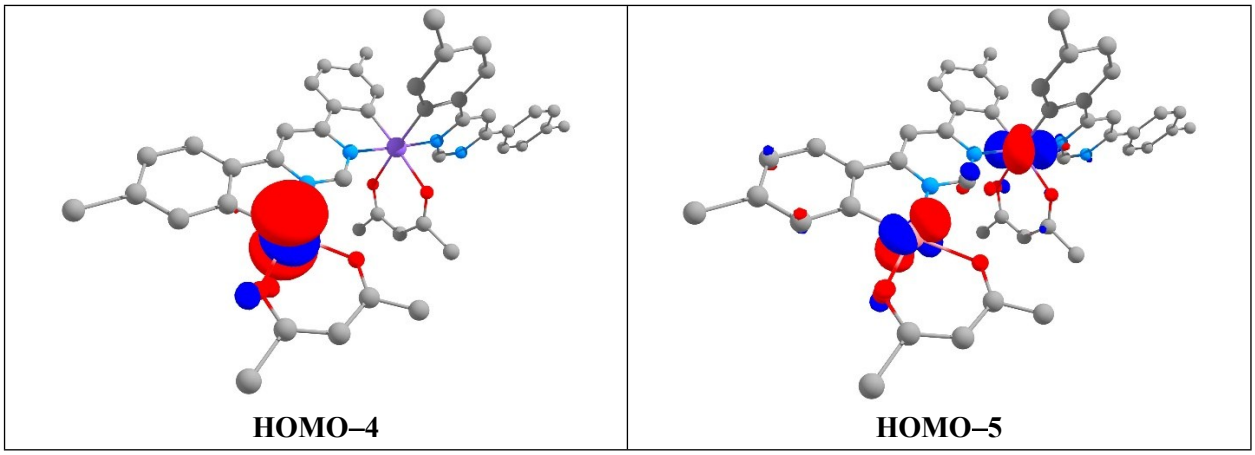
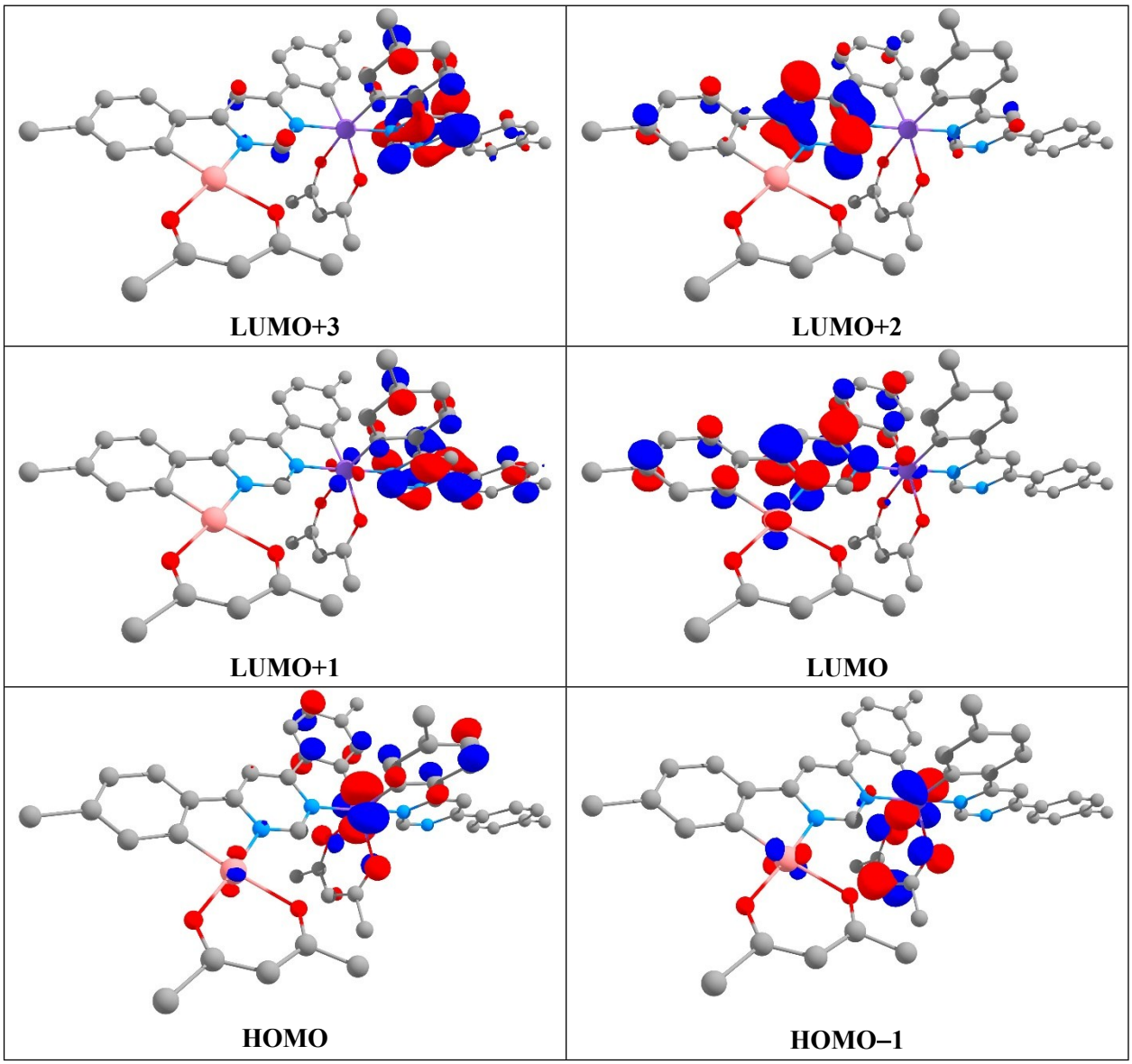
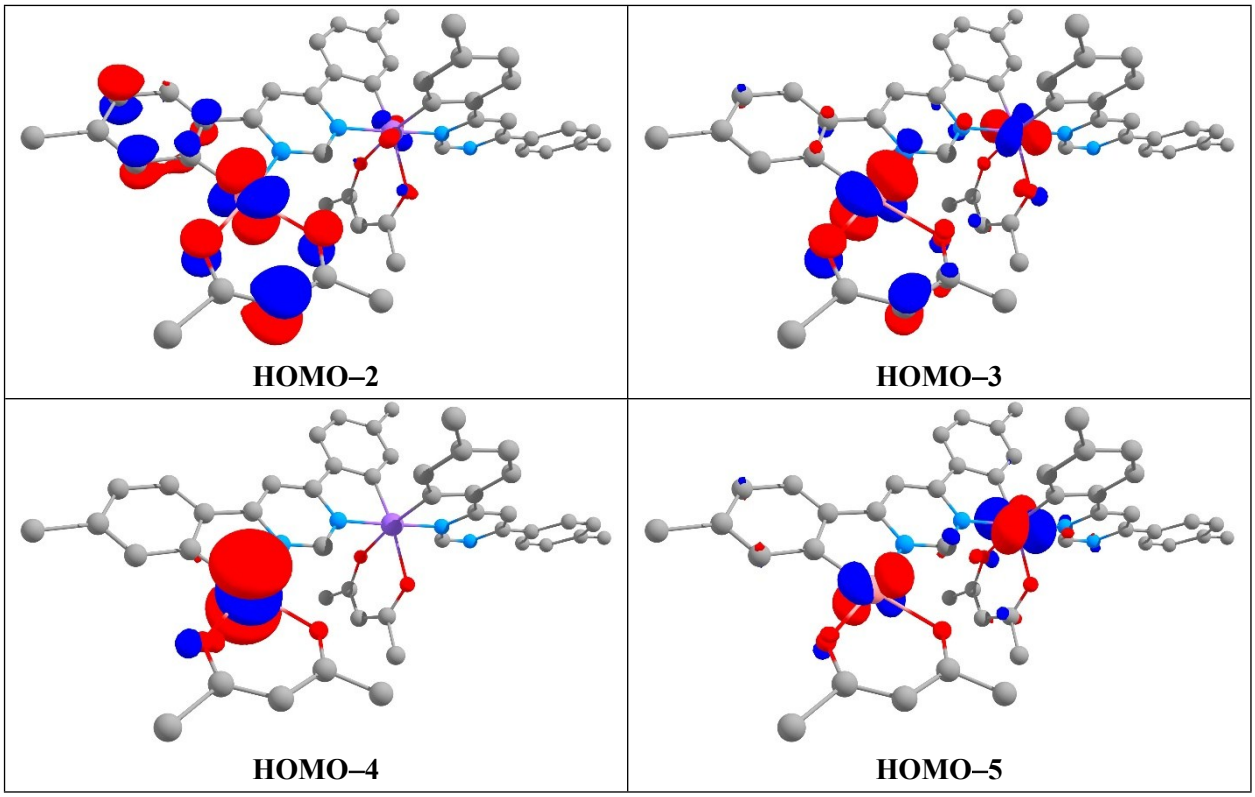


Table S9. Iso-surface contour plots (iso-value = 0.05) of selected orbitals of model complex **2'** at the relaxed T_1 state geometry.





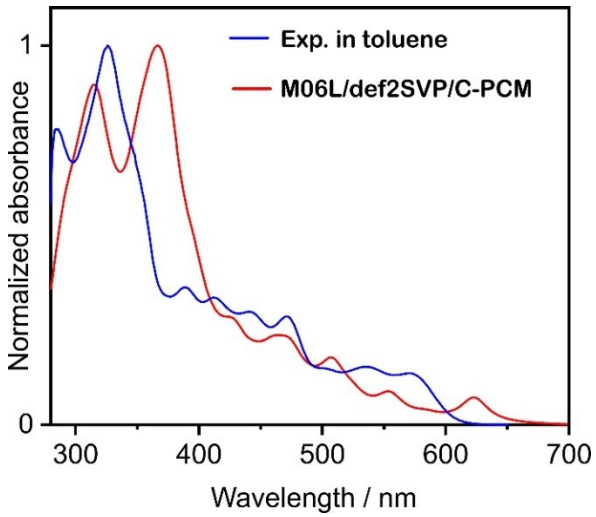


Figure S1. The measured absorption spectrum of compound **2** in toluene (blue), and the TD-DFT-calculated absorption spectrum of model compound **2'** in the optimized ground state geometry (red).

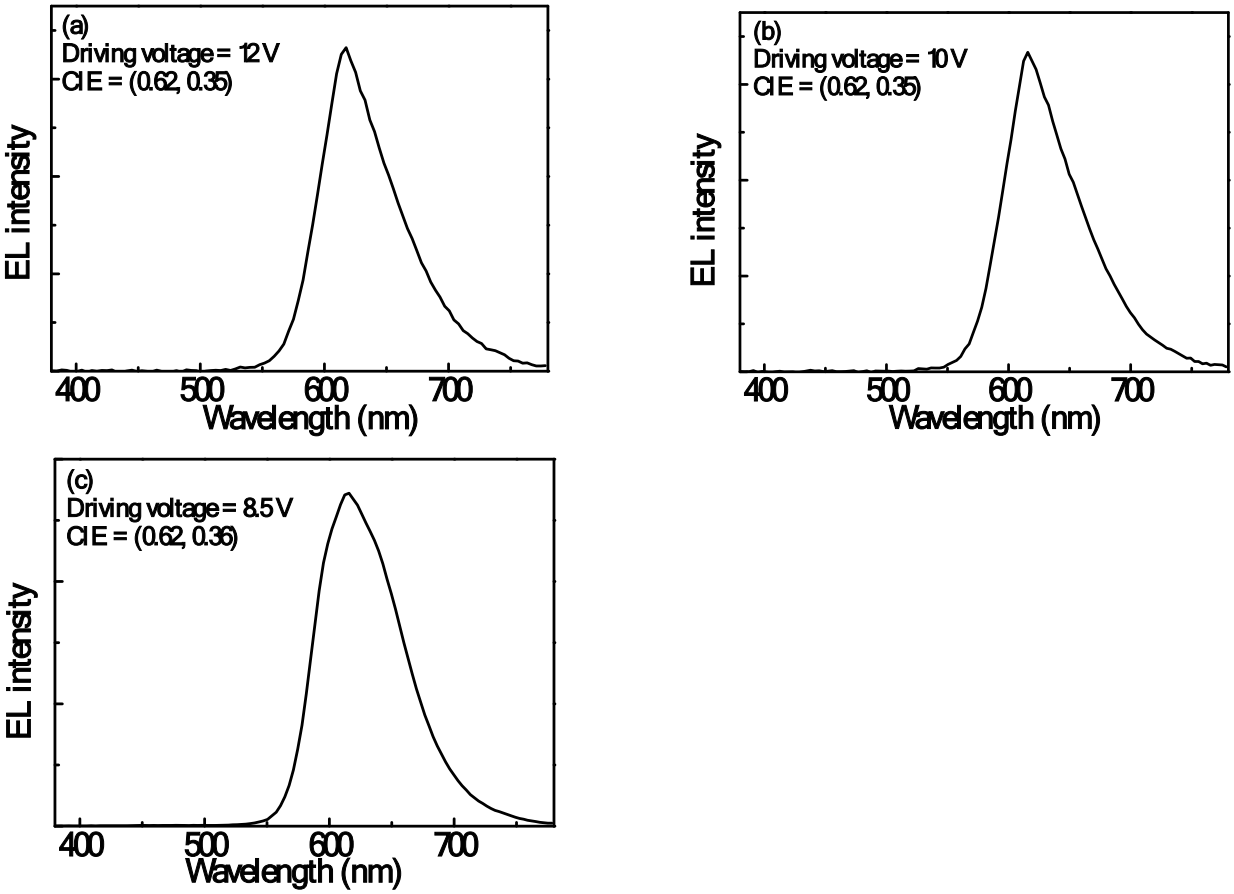


Figure S2. The EL spectrum as a function of drive voltage for the 1 mass% guest concentration LEC. The drive voltage and the corresponding CIE coordinates are identified in the insets.

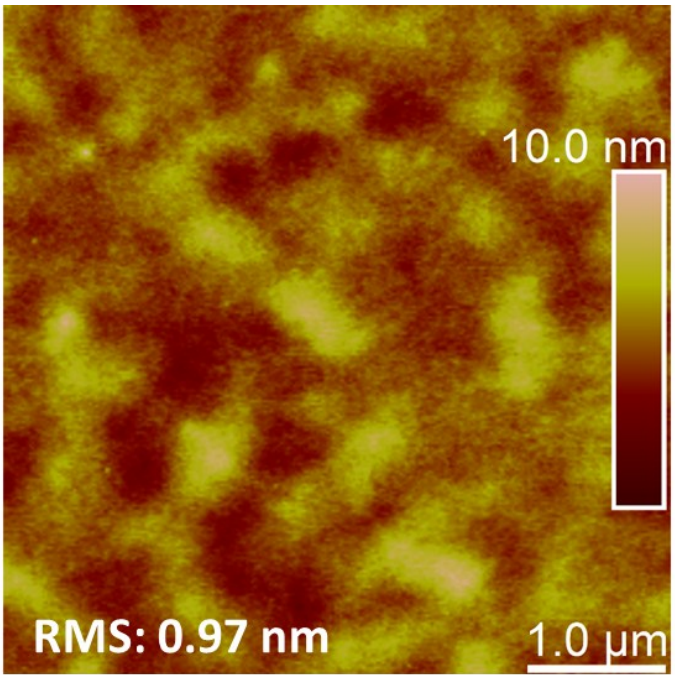


Figure S3. AFM image of the surface morphology of the LEC active material with 1 mass% guest concentration.