Supporting Information to:

Theoretical Design of Porphyrazine Derivatives as Promising Sensitizers for Dye-Sensitized Solar Cells

Jin-Hua Luo,[a] Quan-Song Li*, [a] Li-Na Yang, [a] Zhu-Zhu Sun, [a] Ze-Sheng Li[a,*]

[a] *Key Laboratory of Cluster Science of Ministry of Education, Beijing Key Laboratory of Photoelectronic/ Electrophotonic Conversion Materials, Beijing Key Laboratory for Chemical Power Source and Green Catalysis, School of Chemistry, Beijing Institute of Technology, Beijing 100081, China*

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* Corresponding author at: 5 South Zhongguancun Street Haidian Zone, Beijing 10081, China. Tel.: +86 10 68918670; fax: +86 10 68918670
Email address: liquansong@bit.edu.cn (Q. -S. Li); zeshengli@bit.edu.cn (Z.-S. Li)

1. Cartesian coordinates of optimized structures

The abbreviations used here are consistent with those in the text.

ZnPz

N	-0.82433100	1.72595700	0.07704700
C	-0.16545800	2.91759500	-0.04057000
N	1.15782000	3.10283100	-0.13822000
N	1.82646500	0.77582800	-0.08751100
C	2.06378300	2.11643600	-0.16912900
C	3.50976800	2.33710400	-0.35503600
N	-1.77315600	-0.92828600	0.12296900
N	0.87641200	-1.88141400	-0.02915700
C	-2.96691000	-0.26450500	0.11654800
C	0.20868600	-3.07240100	-0.06923000
C	3.01168200	0.11072300	-0.23205700
C	-4.04584300	-1.24709300	0.07236800
C	1.18359700	-4.14528400	-0.23023400
C	4.07705600	1.09368600	-0.39267100
N	-3.15344900	1.06317200	0.10969900
N	-1.11907100	-3.25642300	-0.01516100
N	3.19396800	-1.21705800	-0.26429200
C	-2.16669600	1.96724600	0.07577900
C	-2.01894500	-2.26940800	0.05870400
C	2.21135800	-2.12253900	-0.18192000
C	-3.47809700	-2.48974700	0.03592900
C	2.42502300	-3.57681100	-0.30076000
Zn	0.04043000	-0.07665200	0.26085500
C	-1.15303700	3.99154600	-0.08980500
C	-2.39359000	3.42235200	-0.01954000
C	-3.74977800	4.06234600	-0.04761700
C	-3.73055900	5.58823700	-0.17520800
H	-4.29517100	3.77071500	0.86092700
H	-4.32665800	3.62516800	-0.87431800
H	-4.75146100	5.98377200	-0.18722100
H	-3.19998700	6.05197300	0.66426200
H	-3.23628400	5.90431600	-1.10095300
C	-4.12370200	-3.84170200	-0.03399500
C	-5.65396500	-3.81413800	-0.08426300
H	-3.78947100	-4.43596300	0.82807800

H	-3.72982800	-4.37304800	-0.91133900
H	-6.05328000	-4.83251400	-0.13218300
H	-6.07366300	-3.32985200	0.80488100
H	-6.01377400	-3.26971900	-0.96481600
C	3.76168800	-4.23748900	-0.45766800
C	4.56994400	-4.27780700	0.85421600
H	4.34344400	-3.69630200	-1.21391800
H	3.61766100	-5.25791500	-0.83110700
H	5.53659100	-4.76786900	0.69266800
H	4.75724400	-3.26508400	1.22514400
H	4.03098200	-4.83249700	1.63033500
C	4.16529500	3.68104500	-0.46398700
C	4.28245100	4.40402200	0.89233300
H	3.58431800	4.30975000	-1.14984200
H	5.16257100	3.56120000	-0.90276700
H	4.76514500	5.37950900	0.76529900
H	3.29299600	4.56625600	1.33158800
H	4.87892800	3.81709500	1.59962200
H	-0.90389700	5.03997400	-0.18386000
H	-5.09701900	-0.99240400	0.05538400
H	0.93109000	-5.19583700	-0.29855700
H	5.12153600	0.84611600	-0.53369700

L1

N	1.97023300	-0.08723200	0.00009400
C	2.53996600	-1.32883600	0.00010800
N	1.91899800	-2.50846900	0.00008700
N	-0.36040700	-1.70224400	0.00001000
C	0.58415000	-2.67177500	0.00003700
C	-0.07558400	-3.99616900	0.00002300
N	0.33041000	2.23153800	0.00007300
N	-1.99062200	0.61138700	0.00002900
C	1.54752000	2.81983100	0.00011400
C	-2.58251600	1.85112800	0.00003000
C	-1.60301200	-2.29477000	-0.00005100
C	1.38204000	4.28881900	0.00013100
C	-4.00707700	1.68502800	-0.00002900
C	-1.41667700	-3.74569400	-0.00005900
N	2.74811200	2.20824000	0.00013000
N	-1.95302300	3.04809700	0.00007200
N	-2.77999100	-1.68056600	-0.00010400
C	2.93015100	0.89016300	0.00012500
C	-0.63764800	3.21481300	0.00008900

C	-2.95072200	-0.34160600	-0.00007200
C	0.03596000	4.51275400	0.00011200
C	-4.26366000	0.31492200	-0.00017100
Zn	-0.01535800	0.26558100	0.00007100
C	4.00331400	-1.16555300	0.00018200
C	5.03035200	-2.09944400	0.00023100
C	4.24752600	0.23755100	0.00018900
C	6.33971600	-1.58898700	0.00030000
C	5.53366800	0.76635700	0.00024400
H	5.73086700	1.83250000	0.00025100
H	4.82767700	-3.16550200	0.00022800
H	-2.22944000	-4.45941200	-0.00009700
H	-4.71930400	2.49686600	-0.00003400
H	-0.48339600	5.46150100	0.00011200
C	0.66321500	-5.30070400	0.00009200
C	-0.23672100	-6.53950900	0.00004700
H	1.33294600	-5.32411500	0.87109800
H	1.33307400	-5.32413900	-0.87081300
H	0.36906700	-7.45141900	0.00011100
H	-0.88130400	-6.56356300	0.88603300
H	-0.88116900	-6.56359700	-0.88603700
C	2.52272700	5.26211100	0.00017800
C	2.09997600	6.73375700	-0.00023200
H	3.16029100	5.05502500	-0.87063600
H	3.15989100	5.05541200	0.87138000
H	2.98051800	7.38434000	-0.00018800
H	1.50242100	6.97630800	-0.88632800
H	1.50204900	6.97670300	0.88550400
C	6.54806000	-0.18578500	0.00030200
C	7.65916400	-2.16964700	0.00036800
C	8.52901100	-1.12864800	0.00040600
O	7.88704100	0.08659800	0.00036900
H	7.91524000	-3.21960900	0.00038700
H	9.60746400	-1.07503600	0.00045900
C	-5.47693500	-0.44372700	-0.00041700
C	-6.77548500	-0.01139900	-0.00038800
H	-5.33056000	-1.51978800	-0.00075400
C	-7.13544400	1.37051800	-0.00002700
N	-7.41084800	2.50200400	0.00026400
C	-7.92492400	-0.94879300	-0.00081200
O	-9.09010700	-0.59537200	-0.00115800
O	-7.55108900	-2.24701400	-0.00078600
H	-8.37305600	-2.77312200	-0.00110400

L2

N	1.75487400	-0.07457000	0.00228700
C	2.32834400	-1.31483800	0.00150200
N	1.71165400	-2.49677200	0.00166700
N	-0.57055400	-1.69865000	0.00243500
C	0.37754400	-2.66488600	0.00215800
C	-0.27735000	-3.99178600	0.00214100
N	0.10486700	2.23790700	0.00219000
N	-2.20997500	0.60862400	0.00255600
C	1.31942000	2.83143800	0.00175500
C	-2.80684800	1.84597600	0.00160200
C	-1.81098200	-2.29590600	0.00246800
C	1.14781800	4.29981100	0.00134100
C	-4.23064000	1.67436200	0.00050900
C	-1.61927100	-3.74618500	0.00234900
N	2.52245800	2.22492000	0.00138600
N	-2.18195800	3.04541100	0.00147400
N	-2.99031600	-1.68639200	0.00230000
C	2.71008100	0.90755200	0.00139000
C	-0.86735800	3.21728100	0.00177300
C	-3.16639300	-0.34806800	0.00208000
C	-0.19914200	4.51804400	0.00134000
C	-4.48188800	0.30322500	0.00086300
Zn	-0.23332600	0.27057800	0.00284900
C	3.79023400	-1.14404100	0.00017200
C	4.82679800	-2.06110900	-0.00121700
C	4.02929500	0.25856900	0.00011000
C	6.14393600	-1.55808800	-0.00274500
C	5.31373000	0.78114300	-0.00135200
H	5.48954300	1.85197600	-0.00144800
H	4.63559000	-3.12987900	-0.00121300
H	-2.42943600	-4.46283400	0.00232300
H	-4.94601300	2.48340400	-0.00036000
H	-0.72258800	5.46453500	0.00098900
C	0.46632500	-5.29348800	0.00180800
C	-0.42895500	-6.53560700	0.00162700
H	1.13628000	-5.31453200	0.87269500
H	1.13611100	-5.31415500	-0.86921700
H	0.18025500	-7.44523000	0.00133600
H	-1.07325100	-6.56232700	0.88773100

H	-1.07346900	-6.56190600	-0.88433200
C	2.28438500	5.27790400	0.00092100
C	1.85533100	6.74775900	0.00018600
H	2.92264700	5.07333000	-0.86997700
H	2.92255400	5.07419900	0.87209600
H	2.73309200	7.40207700	-0.00011500
H	1.25657700	6.98745600	-0.88587000
H	1.25653900	6.98833800	0.88597800
C	6.36270400	-0.14669300	-0.00278500
C	7.38322900	-2.29028700	-0.00451800
C	8.47709600	-1.48360500	-0.00585000
H	7.43680900	-3.37335100	-0.00479100
H	9.51813800	-1.77949900	-0.00730800
S	8.07808200	0.22029500	-0.00501800
C	-5.69221300	-0.46011100	0.00005000
C	-6.99238000	-0.03272300	-0.00265500
H	-5.54172900	-1.53561200	0.00164300
C	-7.35753900	1.34773300	-0.00569100
N	-7.63739400	2.47811300	-0.00833900
C	-8.13827600	-0.97437800	-0.00312900
O	-9.30474100	-0.62527500	-0.00665400
O	-7.75967500	-2.27119900	0.00042800
H	-8.57964700	-2.80040700	-0.00044700

L3

N	-0.30769400	0.29468300	0.00193500
C	0.41734800	-0.86208100	0.00194300
N	-0.03918600	-2.11391500	0.00210700
N	-2.40463600	-1.61506300	0.00191200
C	-1.34036000	-2.45344800	0.00209100
C	-1.81999900	-3.85210500	0.00213500
N	-2.24038700	2.37524600	0.00149500
N	-4.32554300	0.46399900	0.00172200
C	-1.11041600	3.11940000	0.00143000
C	-5.07559900	1.61344400	0.00092500
C	-3.55724700	-2.36583500	0.00181600
C	-1.46952000	4.55452100	0.00124700
C	-6.46710900	1.26033300	-0.00009400
C	-3.18279900	-3.77910100	0.00197500
N	0.15855500	2.67367600	0.00139300
N	-4.61124600	2.88334900	0.00091000
N	-4.80617600	-1.91130500	0.00146400
C	0.51639600	1.38984400	0.00152300

C	-3.32870600	3.22174600	0.00122300
C	-5.15178500	-0.60847200	0.00123400
C	-2.83287900	4.59821900	0.00110900
C	-6.54071200	-0.13045600	0.00004900
Zn	-2.32256900	0.38127300	0.00190100
C	1.84776700	-0.50615500	0.00165900
C	2.98374900	-1.30651600	0.00159300
C	1.90288100	0.91688500	0.00128300
C	4.20470000	-0.62160600	0.00102500
C	3.11962600	1.59026400	0.00064200
H	3.17792500	2.67423500	0.00024800
H	2.92229200	-2.38954200	0.00192000
H	-3.89539200	-4.59272000	0.00191600
H	-7.27981600	1.97153800	-0.00084700
H	-3.47334600	5.46982000	0.00091700
C	-0.91641300	-5.04850900	0.00225100
C	-1.64545300	-6.39496100	0.00201900
H	-0.24955000	-4.98372900	0.87336400
H	-0.24920300	-4.98361600	-0.86858500
H	-0.92455000	-7.21887100	0.00208500
H	-2.28120700	-6.50417500	0.88798000
H	-2.28088900	-6.50403500	-0.88418800
C	-0.46769000	5.66979400	0.00119200
C	-1.08074600	7.07289900	0.00121000
H	0.19135900	5.54888100	-0.86984800
H	0.19143600	5.54889200	0.87217400
H	-0.29324300	7.83340400	0.00118300
H	-1.70509300	7.23488900	-0.88481100
H	-1.70503200	7.23488400	0.88727500
C	4.27147700	0.80346400	0.00048400
C	6.41730300	-0.12114800	-0.00011800
C	7.77130400	-0.28084500	-0.00080900
C	8.49732300	-1.58994600	-0.00064300
C	9.98916300	0.19235200	-0.00248600
C	9.91610700	-1.22059300	-0.00179300
C	11.21873300	0.85009300	-0.00368700
C	11.07846000	-1.99557800	-0.00226500
C	12.37056100	0.05830100	-0.00416500
H	11.28192700	1.93366200	-0.00424600
C	12.31200800	-1.34692600	-0.00345900
H	11.00964300	-3.07954300	-0.00171800
H	13.34052200	0.54781000	-0.00511100
H	13.23182800	-1.92307800	-0.00385700
N	5.48363200	-1.14167800	0.00078300

N	8.70472500	0.72875700	-0.00180500
H	5.75003100	-2.11883400	0.00099800
H	8.44692700	1.70777600	-0.00211500
O	7.95297800	-2.69759300	0.00018400
C	5.69183800	1.17703700	-0.00034400
O	6.22415900	2.29197400	-0.00109700
C	-7.64312500	-1.04367700	-0.00079900
C	-8.98697000	-0.78690800	-0.00336000
H	-7.35487100	-2.09079600	0.00055000
C	-9.52658100	0.53528800	-0.00593200
N	-9.94928500	1.62031500	-0.00803400
C	-10.00251900	-1.86866000	-0.00422100
O	-11.20399500	-1.67230700	-0.00757600
O	-9.45949300	-3.10545600	-0.00086600
H	-10.20383900	-3.73659300	-0.00196700

L4

N	1.80269800	-0.02154200	-0.00129500
C	2.39036600	-1.25456000	-0.00092200
N	1.79331800	-2.44475200	-0.00095600
N	-0.50050900	-1.68268300	-0.00140600
C	0.46154400	-2.63463100	-0.00121300
C	-0.17178200	-3.97119200	-0.00101600
N	0.11066700	2.26385000	-0.00121000
N	-2.17812400	0.59778100	-0.00138100
C	1.31436800	2.87841100	-0.00116400
C	-2.79494000	1.82458800	-0.00087200
C	-1.73182200	-2.29968500	-0.00142700
C	1.11842600	4.34365000	-0.00107200
C	-4.21636800	1.62995400	-0.00033200
C	-1.51752900	-3.74639000	-0.00119500
N	2.52738500	2.29178800	-0.00097700
N	-2.18961100	3.03378700	-0.00079000
N	-2.92077300	-1.70900500	-0.00140200
C	2.73761700	0.97887500	-0.00091200
C	-0.87816100	3.22716400	-0.00099500
C	-3.11903000	-0.37436900	-0.00127200
C	-0.23201300	4.53888800	-0.00088300
C	-4.44517500	0.25539800	-0.00066000
Zn	-0.19644700	0.29177600	-0.00150900
H	-2.31639600	-4.47560000	-0.00106500
H	-4.94453100	2.42748500	0.00014500
H	-0.77173700	5.47615900	-0.00070100

C	0.59205600	-5.26114300	-0.00058200
C	-0.28406000	-6.51681600	0.00108600
H	1.26271300	-5.27095400	0.86992500
H	1.26140900	-5.27235200	-0.87208900
H	0.33918100	-7.41684600	0.00138600
H	-0.92723700	-6.55253000	0.88765300
H	-0.92853400	-6.55403200	-0.88447700
C	2.23820700	5.34089900	-0.00120500
C	1.78397400	6.80315900	0.00085700
H	2.87876200	5.14861300	-0.87322000
H	2.88068700	5.14669900	0.86894900
H	2.65045100	7.47227800	0.00059800
H	1.18023700	7.03389600	-0.88417800
H	1.18221400	7.03196900	0.88773400
C	3.85190200	-1.06209400	-0.00025400
C	4.89597200	-1.95456200	0.00041200
C	6.22293200	-1.43882900	0.00124900
C	6.43846600	-0.01868000	0.00136500
C	5.33817500	0.88030700	0.00059900
C	4.06979900	0.35293500	-0.00019200
H	7.26653300	-3.34715600	0.00202000
H	4.72413100	-3.02673800	0.00038900
C	7.37463900	-2.26646000	0.00207400
C	7.78452100	0.44177800	0.00233800
H	5.50592700	1.95346100	0.00070600
H	7.96918200	1.51639500	0.00246300
C	8.62515700	-1.68978900	0.00298300
H	9.51815600	-2.31024400	0.00365800
N	8.84333000	-0.34412400	0.00313700
C	-5.64326400	-0.52792700	-0.00048000
C	-6.94960900	-0.12096700	0.00145700
H	-5.47546400	-1.60086100	-0.00189700
C	-7.33614900	1.25374500	0.00414700
N	-7.63310000	2.37970000	0.00641700
C	-8.08113400	-1.08050900	0.00146200
O	-9.25255600	-0.74898100	0.00450000
O	-7.68222500	-2.37100800	-0.00228700
H	-8.49351500	-2.91348300	-0.00168500

L5

N	-1.00527500	0.10690900	0.00056900
C	-1.64551000	-1.10083300	0.00055800

N	-1.09726300	-2.31510600	0.00053000
N	1.22682000	-1.65059700	0.00055600
C	0.22523700	-2.55982700	0.00052400
C	0.80106400	-3.92310600	0.00039600
N	0.78529600	2.31771700	0.00056000
N	3.00134300	0.55495200	0.00035900
C	-0.38981900	2.98317700	0.00057400
C	3.67096200	1.75495100	0.00016500
C	2.43175900	-2.32011400	0.00042700
C	-0.13164600	4.43872300	0.00051400
C	5.08077700	1.50026500	-0.00021500
C	2.15478000	-3.75660100	0.00035300
N	-1.62785200	2.44984700	0.00061000
N	3.11660400	2.98958600	0.00021700
N	3.64387400	-1.78259600	0.00029500
C	-1.89490000	1.14812900	0.00059900
C	1.81589900	3.23861200	0.00039300
C	3.89992500	-0.45595900	0.00024100
C	1.22573900	4.57642500	0.00038700
C	5.25066100	0.11564100	-0.00021000
Zn	1.00782900	0.33473700	0.00054700
H	2.92169000	-4.51943700	0.00022900
H	5.84243600	2.26587500	-0.00042200
H	1.80476900	5.49005500	0.00028100
C	-0.01805200	-5.17861500	0.00033000
C	0.80251400	-6.47134500	-0.00047300
H	-0.68839100	-5.15968100	-0.87030800
H	-0.68759900	-5.16029200	0.87159900
H	0.14067500	-7.34341900	-0.00053500
H	1.44383900	-6.53550500	-0.88680200
H	1.44453100	-6.53617400	0.88530400
C	-1.20828300	5.48228500	0.00061300
C	-0.69311300	6.92423600	-0.00037400
H	-1.85703100	5.31699600	0.87209000
H	-1.85804800	5.31610900	-0.86992300
H	-1.53080600	7.62906300	-0.00029200
H	-0.08074100	7.12890000	0.88518000
H	-0.08164500	7.12799600	-0.88676000
C	-3.09455400	-0.84787300	0.00051800
C	-4.17503900	-1.68710500	0.00043700
C	-5.48560400	-1.11525600	0.00037900
C	-5.65158700	0.32866000	0.00043800
C	-4.49002100	1.16863400	0.00053400
C	-3.25513400	0.58185400	0.00056000

H	-6.56248100	-2.98351200	0.00018700
H	-4.05453500	-2.76665500	0.00038900
C	-6.64433500	-1.89888400	0.00024700
H	-4.62378800	2.24519100	0.00055600
C	-9.23893600	0.78543800	0.00016400
C	-9.12592200	-2.03761600	0.00001300
C	-10.38866200	0.03717900	0.00001100
H	-9.26303700	1.87067800	0.00022000
C	-10.33396200	-1.38863600	-0.00006700
H	-9.07619600	-3.12343300	-0.00005000
H	-11.35678900	0.52992900	-0.00005500
H	-11.25926800	-1.95713600	-0.00019200
C	-7.95880300	0.14979400	0.00024700
C	-7.90584800	-1.29488500	0.00017000
N	-6.85616100	0.92175700	0.00037600
C	6.41335300	-0.71789600	-0.00049600
C	7.73669000	-0.36798300	-0.00166100
H	6.19865000	-1.78249800	0.00011800
C	8.18277500	0.98841200	-0.00288300
N	8.52925600	2.10019100	-0.00386600
C	8.82520300	-1.37524800	-0.00192000
O	10.01028000	-1.09572900	-0.00349600
O	8.37078400	-2.64769100	0.00006700
H	9.15822800	-3.22419900	-0.00018200

L6

N	1.80595600	-0.01987300	-0.00049800
C	2.39285900	-1.25252400	-0.00049400
N	1.79723400	-2.44338700	-0.00039700
N	-0.49640400	-1.68199200	-0.00015500
C	0.46638700	-2.63482300	-0.00030200
C	-0.16703500	-3.97106400	-0.00030000
N	0.11390000	2.26498800	-0.00040500
N	-2.17377100	0.59802400	-0.00002100
C	1.31805000	2.88131300	-0.00048200
C	-2.79018300	1.82422400	0.00012300
C	-1.72612700	-2.29891300	-0.00006200
C	1.12091000	4.34574800	-0.00010200
C	-4.21414600	1.62830800	0.00061200
C	-1.51286500	-3.74550100	-0.00018700
N	2.53011200	2.29372800	-0.00073600
N	-2.18706800	3.03206000	0.00010500

N	-2.91649200	-1.70758300	0.00016500
C	2.73832300	0.98092100	-0.00077800
C	-0.87403600	3.22681700	-0.00010000
C	-3.11424000	-0.37460600	0.00024100
C	-0.23013200	4.53913700	0.00003300
C	-4.44213200	0.25576200	0.00054900
Zn	-0.19323200	0.29258800	-0.00044700
H	-2.31205200	-4.47424100	-0.00010500
H	-4.94190300	2.42618900	0.00093000
H	-0.77107600	5.47562000	0.00036000
C	0.59608600	-5.26148700	-0.00056500
C	-0.28082900	-6.51660500	0.00032400
H	1.26668700	-5.27194100	0.86995900
H	1.26530600	-5.27236100	-0.87218500
H	0.34213200	-7.41677700	0.00023600
H	-0.92405600	-6.55247800	0.88682500
H	-0.92502500	-6.55303600	-0.88544800
C	2.23911000	5.34477700	0.00009600
C	1.78246000	6.80627400	0.00074800
H	2.88062400	5.15284200	-0.87126500
H	2.88093200	5.15216500	0.87107600
H	2.64800400	7.47653600	0.00090800
H	1.17936900	7.03550600	-0.88509000
H	1.17960300	7.03477400	0.88692500
C	3.85366200	-1.05911400	-0.00056600
C	4.90093700	-1.95255900	-0.00035100
C	6.21433000	-1.42117700	-0.00041300
C	6.43220200	-0.01277000	-0.00085000
C	5.34045600	0.89025600	-0.00109400
C	4.07234800	0.35477200	-0.00085100
H	7.29433900	-3.31362000	0.00054500
H	4.73464500	-3.02548000	-0.00007000
C	7.38809300	-2.22876700	0.00007300
C	7.79501800	0.40282300	-0.00093400
H	5.50553000	1.96337800	-0.00138200
H	8.03301200	1.46546300	-0.00146800
N	8.61753500	-1.76494000	0.00006700
N	8.82700400	-0.41056400	-0.00054400
C	-5.64042700	-0.52911800	0.00092500
C	-6.94583200	-0.12210800	0.00111400
H	-5.47194000	-1.60193500	0.00107900
C	-7.33201000	1.25280900	0.00102100
N	-7.62791200	2.37897500	0.00093100
C	-8.07818400	-1.08189500	0.00152100

O	-9.24891800	-0.74882100	0.00210600
O	-7.67934000	-2.37174900	0.00124500
H	-8.49006500	-2.91516100	0.00147900

L7

N	1.40334900	0.02432700	-0.00058200
C	2.00542700	-1.20026500	-0.00072800
N	1.39971700	-2.39231200	-0.00072600
N	-0.89684600	-1.63858300	-0.00030500
C	0.07289400	-2.58799800	-0.00044500
C	-0.55830400	-3.92635900	-0.00008900
N	-0.29177800	2.30470000	-0.00051700
N	-2.57152100	0.63658100	-0.00013600
C	0.91654700	2.91875200	-0.00027900
C	-3.18888600	1.86146500	-0.00019900
C	-2.12040200	-2.25790900	0.00029800
C	0.71836100	4.38420000	0.00000500
C	-4.61623400	1.66318400	0.00006800
C	-1.90474300	-3.70399800	0.00045600
N	2.12484400	2.33156900	-0.00022200
N	-2.59161100	3.06921800	-0.00030300
N	-3.31505700	-1.66789800	0.00068100
C	2.34513000	1.01480700	-0.00038000
C	-1.27527400	3.26457400	-0.00033400
C	-3.51107000	-0.33741400	0.00043300
C	-0.63271500	4.57740800	-0.00005200
C	-4.84224500	0.29310300	0.00059400
Zn	-0.58659200	0.33261900	-0.00056800
H	-2.70205400	-4.43479600	0.00087300
H	-5.34381100	2.46128000	0.00011800
H	-1.17374900	5.51381900	0.00012300
C	0.20390500	-5.21727100	-0.00029400
C	-0.67381500	-6.47207000	0.00009700
H	0.87349500	-5.22910400	0.87104500
H	0.87283900	-5.22919400	-0.87213500
H	-0.05132000	-7.37256000	-0.00016500
H	-1.31707600	-6.50779700	0.88654200
H	-1.31784300	-6.50781000	-0.88579000
C	1.83335100	5.38668000	0.00032600
C	1.37242100	6.84702700	0.00099400
H	2.47503400	5.19763000	-0.87157500

H	2.47519600	5.19687500	0.87193900
H	2.23609300	7.51968700	0.00123600
H	0.76882500	7.07443400	-0.88492100
H	0.76893700	7.07364400	0.88718900
C	6.57055000	2.76275900	0.00166200
C	5.26079200	2.32987100	0.00083200
C	4.99412000	0.94069400	0.00027000
C	6.10647900	0.04615500	0.00050900
C	7.59739900	1.79863700	0.00186800
C	3.67486000	0.37973700	-0.00031300
C	5.88461900	-1.40307000	-0.00003500
C	4.55540800	-1.92351700	-0.00068200
C	3.46439900	-0.99328200	-0.00066900
C	4.39401300	-3.32877300	-0.00125200
H	3.39267600	-3.74251200	-0.00175800
C	5.51429700	-4.13382600	-0.00112300
C	6.78274700	-3.52128300	-0.00038500
H	6.81450600	3.82050700	0.00216500
H	4.42920200	3.02434300	0.00066100
H	8.63941800	2.11631500	0.00253600
H	5.43058800	-5.21609700	-0.00155900
H	7.68184500	-4.13637900	-0.00022400
N	7.38477400	0.49080900	0.00128800
N	6.97158400	-2.20984100	0.00014500
C	-6.04021600	-0.49408300	0.00164900
C	-7.34518400	-0.08750000	0.00010600
H	-5.87044100	-1.56666100	0.00386300
C	-7.73184700	1.28755400	-0.00383600
N	-8.02762500	2.41362800	-0.00734100
C	-8.47820600	-1.04784200	0.00204800
O	-9.64838400	-0.71393500	0.00078300
O	-8.07863900	-2.33717500	0.00545300
H	-8.88871700	-2.88160700	0.00637100

L8

N	-1.80937900	-0.01645200	0.00112900
C	-2.39718900	-1.24888800	0.00070900
N	-1.80249100	-2.43941200	0.00076300
N	0.49197300	-1.68065900	0.00128000
C	-0.47137200	-2.63195000	0.00102400
C	0.16018400	-3.96890000	0.00095800

N	-0.11453200	2.26673500	0.00126100
N	2.17205400	0.59777900	0.00153200
C	-1.31768400	2.88346500	0.00101500
C	2.78991000	1.82342600	0.00122600
C	1.72174200	-2.29892500	0.00124300
C	-1.11951700	4.34805400	0.00084100
C	4.21245100	1.62668700	0.00091600
C	1.50637000	-3.74524100	0.00106300
N	-2.53077100	2.29758500	0.00074800
N	2.18700700	3.03268600	0.00114600
N	2.91207900	-1.70909500	0.00123800
C	-2.74138000	0.98513400	0.00070300
C	0.87497500	3.22809500	0.00117200
C	3.11160000	-0.37578100	0.00127900
C	0.23146300	4.54087200	0.00093900
C	4.43940400	0.25286100	0.00090400
Zn	0.19077100	0.29417300	0.00151400
H	2.30453500	-4.47523500	0.00100500
H	4.94119000	2.42371700	0.00065000
H	0.77285400	5.47717200	0.00080600
C	-0.60491300	-5.25811700	0.00076800
C	0.27011700	-6.51465100	0.00012800
H	-1.27519200	-5.26764900	-0.87000800
H	-1.27468000	-5.26821300	0.87194000
H	-0.35420200	-7.41389300	-0.00001400
H	0.91361400	-6.55146700	-0.88619100
H	0.91406200	-6.55207100	0.88609500
C	-2.23725000	5.34760100	0.00062200
C	-1.77992400	6.80890200	-0.00105900
H	-2.87848500	5.15659000	0.87241300
H	-2.87966300	5.15488500	-0.86990700
H	-2.64504200	7.47974600	-0.00120400
H	-1.17623300	7.03829000	0.88435400
H	-1.17725100	7.03654200	-0.88761500
C	-3.85960400	-1.05505100	0.00007100
C	-4.90246300	-1.95047200	-0.00059900
C	-6.22454900	-1.42918300	-0.00134400
C	-6.43665300	-0.01095200	-0.00135300
C	-5.34236300	0.89210000	-0.00064200
C	-4.07509900	0.36065000	0.00005500
H	-4.75007600	-3.02431100	-0.00062800
C	-7.79246300	0.40914500	-0.00219000
H	-5.51073500	1.96512700	-0.00068400
H	-8.02541700	1.47430400	-0.00224100

C	-8.48515600	-1.75674000	-0.00283400
N	-7.28346500	-2.29207700	-0.00209200
N	-8.80755300	-0.43179700	-0.00293200
H	-9.32977700	-2.44284900	-0.00345000
C	5.63688800	-0.53264100	0.00044900
C	6.94319400	-0.12694900	-0.00135200
H	5.46774600	-1.60538200	0.00159600
C	7.33100700	1.24759300	-0.00318600
N	7.62836500	2.37336300	-0.00438200
C	8.07422400	-1.08789300	-0.00212800
O	9.24558400	-0.75663800	-0.00555000
O	7.67399000	-2.37750100	0.00104400
H	8.48432800	-2.92148300	-0.00050400

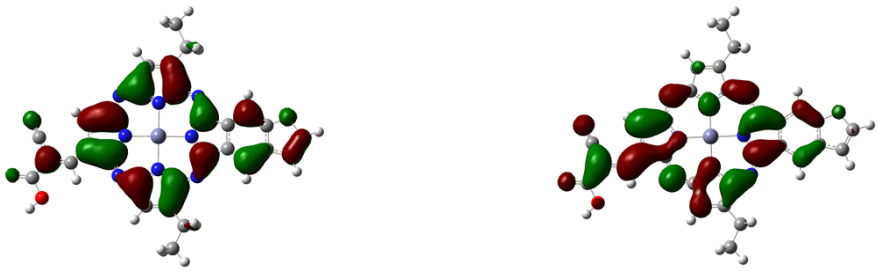
L9

N	-1.57361400	0.12257500	0.00237300
C	-2.21789400	-1.08223800	0.00185900
N	-1.67700900	-2.29924000	0.00191400
N	0.64882300	-1.64124000	0.00225600
C	-0.35608800	-2.55024300	0.00213500
C	0.21725900	-3.91296700	0.00202400
N	0.21336400	2.32949700	0.00209900
N	2.42411300	0.56301500	0.00201800
C	-0.96339400	2.99712400	0.00189700
C	3.09396000	1.76056700	0.00121600
C	1.84915500	-2.31188800	0.00198700
C	-0.70188800	4.45193700	0.00135100
C	4.50793200	1.50210700	0.00022600
C	1.57203300	-3.74745700	0.00188700
N	-2.19979700	2.46390800	0.00181200
N	2.54542400	2.99457400	0.00112100
N	3.06488600	-1.77322300	0.00165500
C	-2.46536800	1.16018100	0.00186500
C	1.24202200	3.24683900	0.00151800
C	3.32071300	-0.45069000	0.00151300
C	0.65614600	4.58639200	0.00110900
C	4.67517100	0.12075900	0.00042600
Zn	0.43205300	0.34499600	0.00251300
H	2.33800000	-4.51115200	0.00167700
H	5.27020400	2.26714500	-0.00051600
H	1.23742800	5.49849700	0.00059200

C	-0.60220800	-5.16836900	0.00202100
C	0.21800500	-6.46132600	0.00083200
H	-1.27270900	-5.14903900	-0.86843600
H	-1.27143500	-5.14987100	0.87348800
H	-0.44450400	-7.33281800	0.00092500
H	0.85883900	-6.52579700	-0.88582600
H	0.86014500	-6.52662600	0.88648300
C	-1.77502100	5.49909900	0.00104100
C	-1.25520900	6.93929400	-0.00151300
H	-2.42364200	5.33659600	0.87316300
H	-2.42549700	5.33412300	-0.86921300
H	-2.09068200	7.64671300	-0.00163900
H	-0.64185100	7.14285900	0.88355600
H	-0.64368800	7.14031600	-0.88843100
C	-3.66722900	-0.82055600	0.00094500
C	-4.76150300	-1.67269500	-0.00022600
C	-6.02747600	-1.07933500	-0.00140200
C	-6.20661100	0.32679000	-0.00126900
C	-5.07822500	1.16935000	-0.00002200
C	-3.82126500	0.58939600	0.00100600
H	-4.66047900	-2.75217600	-0.00041600
C	-7.56062900	0.82144600	-0.00265800
H	-5.20262600	2.24791100	-0.00002300
H	-7.72082400	1.89623400	-0.00247200
C	-8.42092300	-1.47427400	-0.00455300
O	-7.10134800	-1.92210900	-0.00286800
O	-9.29363900	-2.31565200	-0.00614600
C	-8.61158100	-0.03077400	-0.00426600
H	-9.63943700	0.31213600	-0.00544100
C	5.83749900	-0.71645600	-0.00028800
C	7.15995600	-0.36784300	-0.00266900
H	5.62091800	-1.78067900	0.00101000
C	7.60684700	0.98876000	-0.00519100
N	7.95254100	2.10062700	-0.00730900
C	8.24858400	-1.37695000	-0.00331100
O	9.43300900	-1.09647900	-0.00624300
O	7.79252400	-2.64785200	-0.00039100
H	8.57820200	-3.22685400	-0.00120200

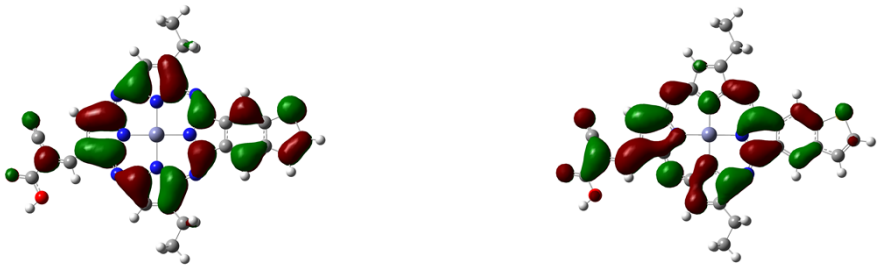
2. Frontier molecular orbitals of zinc porphyrazine derivatives calculated at the B3LYP/6-31G(d) level in chloroform solution.

HOMO LUMO

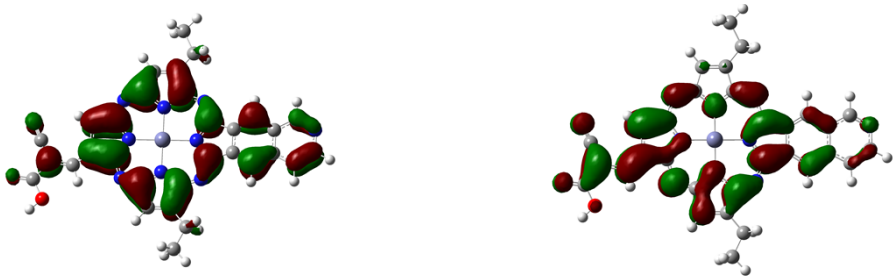


L1

HOMO LUMO



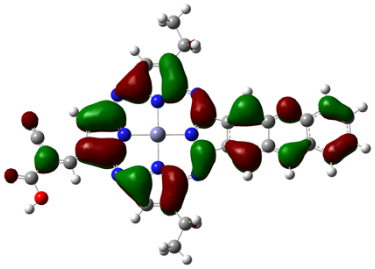
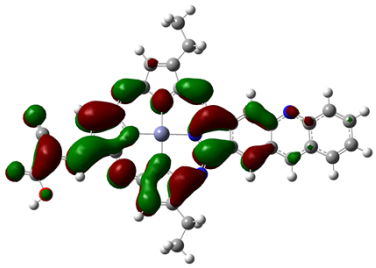
L2



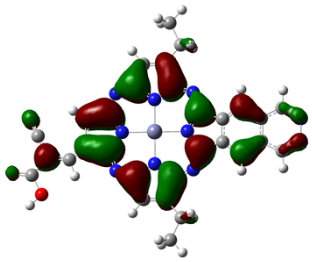
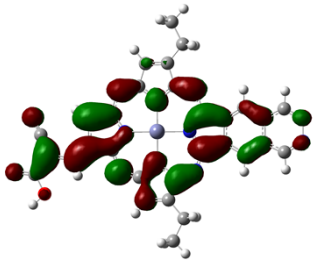
L4

Fig. S1(a). The HOMO and LUMO of L1, L2, and L4.

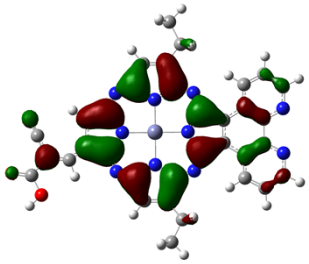
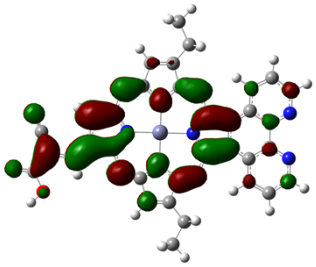
HOMO LUMO

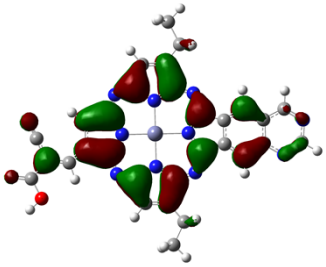
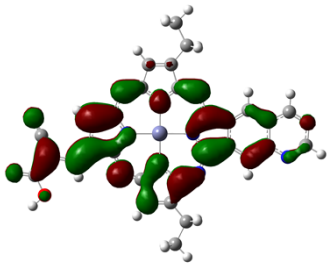
L5

L6

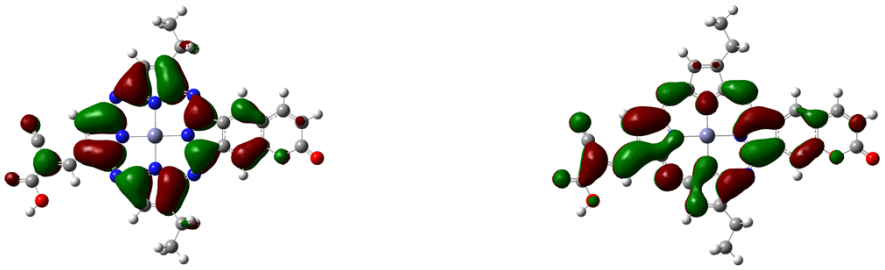
L7

L8

Fig. S1(b). The HOMO and LUMO of L5, L6, L7, and L8.

HOMO LUMO



L9

Fig. S1(c). The HOMO and LUMO of L9.

3. The computational details of E_{OX}^{dye}

The E_{OX}^{dye} is obtained by the computational method which is proposed by De Angelis et al.[1] The rigorous way to obtain the ground state oxidation potential E_{OX}^{dye} is to compute the free energy difference between the neutral and the oxidized ground state species, $E_{OX}^{dye} = (G^0 - G^+)_{GS}$. Herein G^0 and G^+ are free energies of the ground state in neutral and oxidized forms, respectively. The Gibbs free energy in solution of a species i (G_{solv}^i) is defined as $G_{solv}^i = G_{vac}^i + \Delta G_{solv}^i$, where G_{vac}^i is the Gibbs free energy in gas phase and ΔG_{solv}^i is the free energy of solvation. G_{vac}^i is obtained by performing a single-point calculation at the optimized geometry in vacuo, followed by frequency calculations in order to include the vibrational contribution to the total partition function. ΔG_{solv}^i is obtained by a single-point calculation in solution and a

reference calculation in gas phase at the geometry optimized in solution.

Geometry optimization of the neutral and oxidized sensitizers were carried out in gas phase and in chloroform, that is the solvent experimentally employed for the electrochemical measures, by using the B3LYP exchange-correlation functional and a 6-31G(d) basis set for C, H, O, N, S and LANL2DZ basis set for zinc atom. Solvation effects were taken into account by means of the C-PCM salvation model as implemented in Gaussian 09 (G09).

1. M. Pastore, S. Fantacci and F. De Angelis, *J. Phys. Chem. C*, 2010, **114**, 22742.