

Supplementary Information

Digital Discovery of Large-Scale Optoelectronic Materials via MPNICE Machine-Learning Force Fields

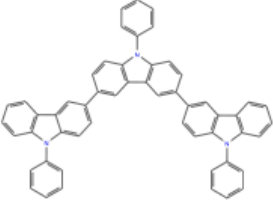
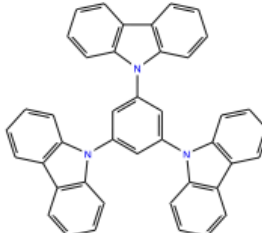
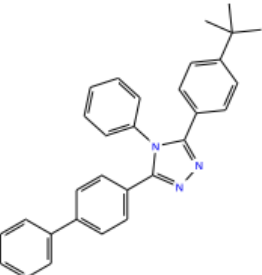
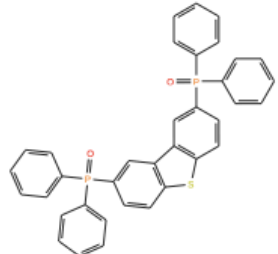
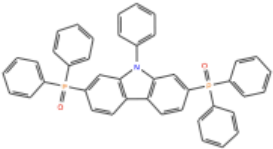
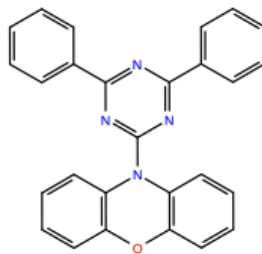
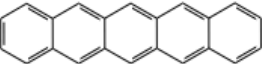
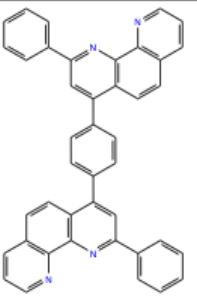
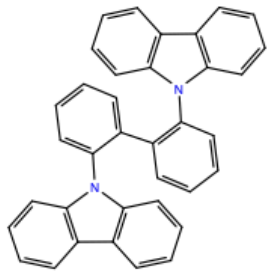

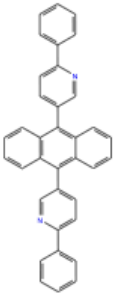
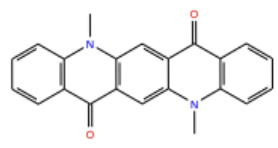
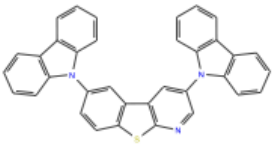
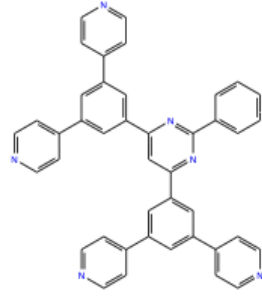
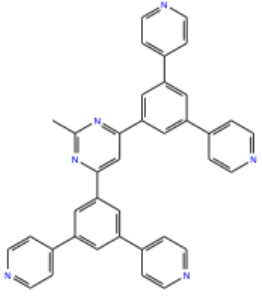
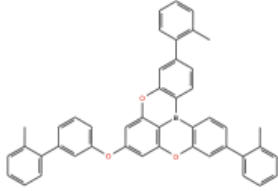
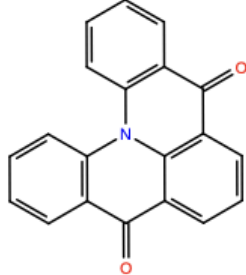
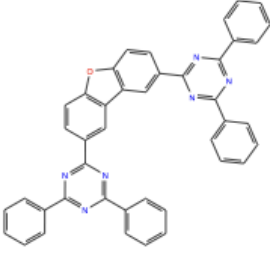
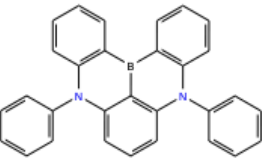
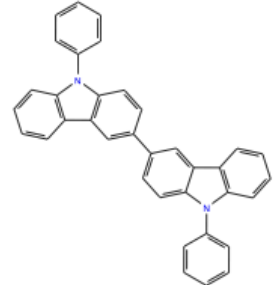
Hadi Abroshan,* H. Shaun Kwak, David J. Giesen, John L. Weber, and Mathew D.
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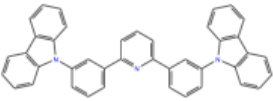
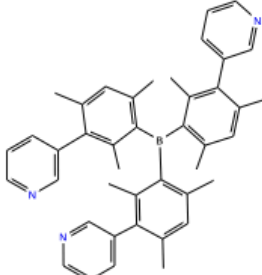
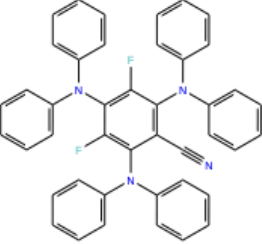
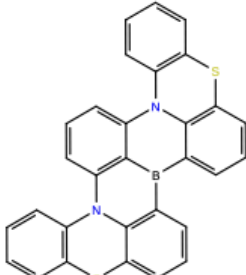
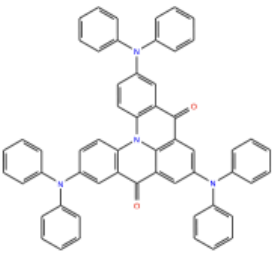
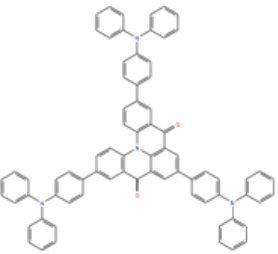
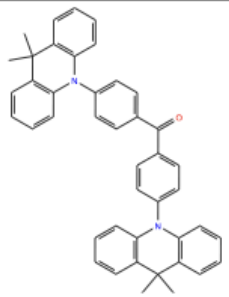
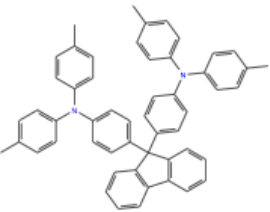
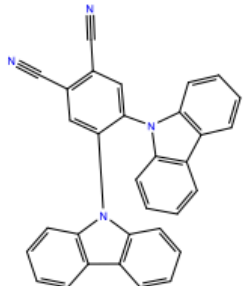
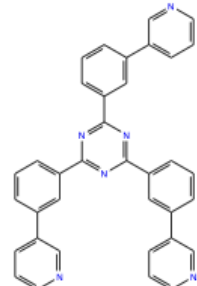
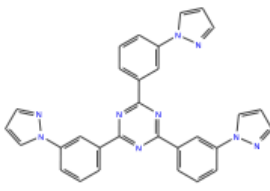
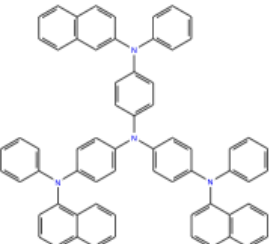
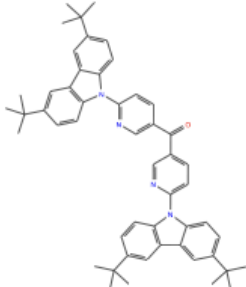
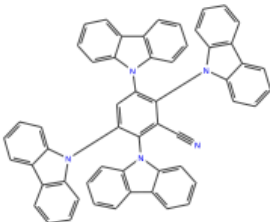
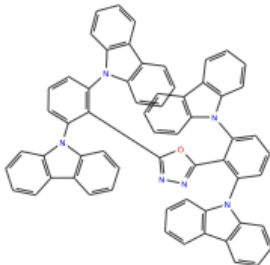
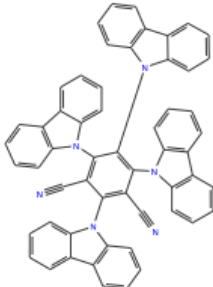
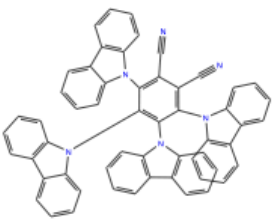
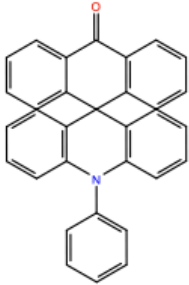
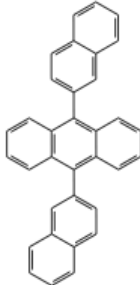
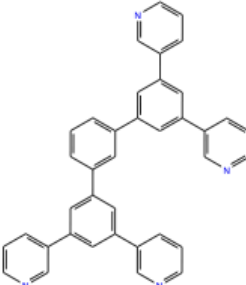
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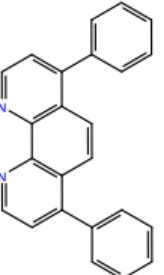
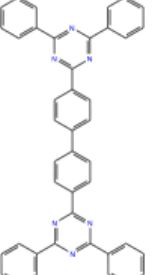
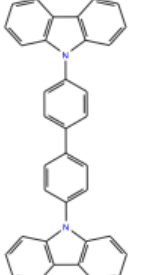
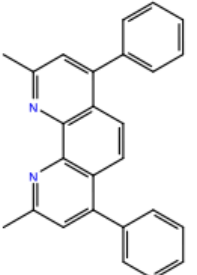
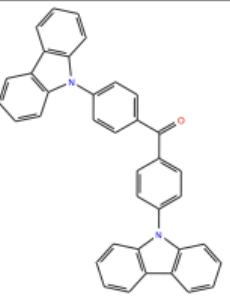
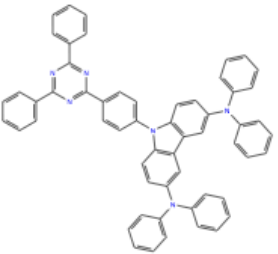
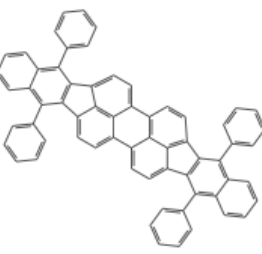
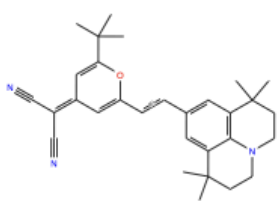
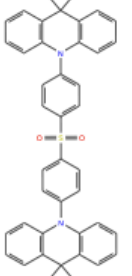
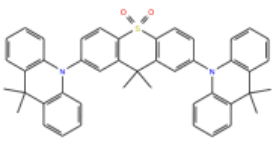
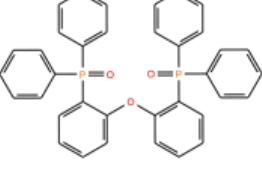
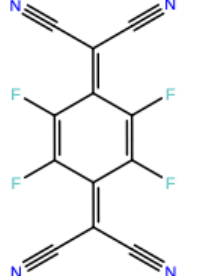
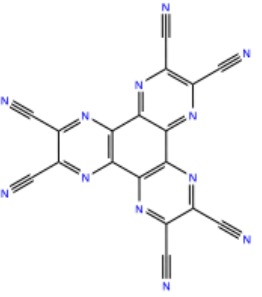
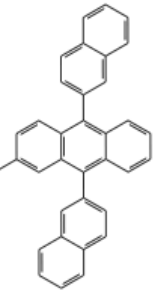
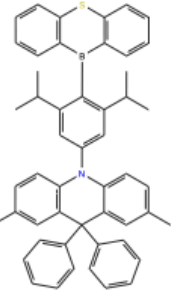
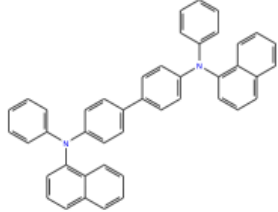
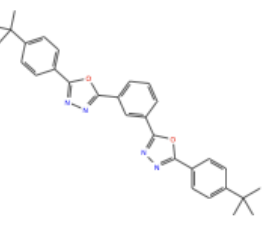
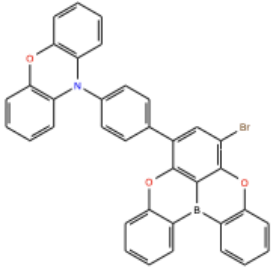
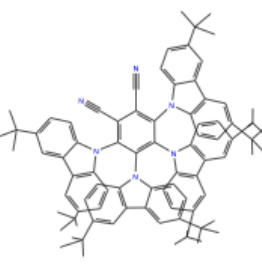
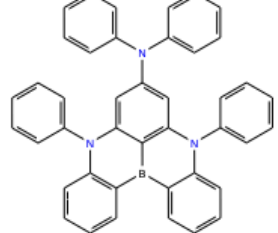
* **Correspondence:** Hadi Abroshan, hadi.abroshan@schrodinger.com

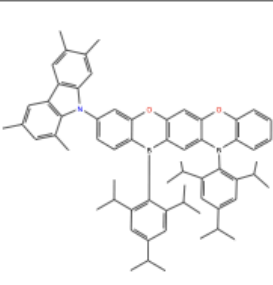
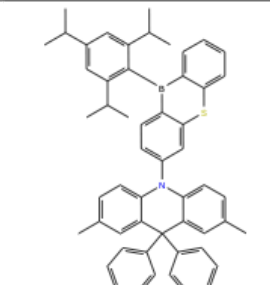
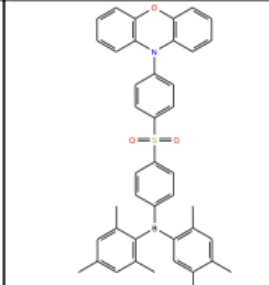
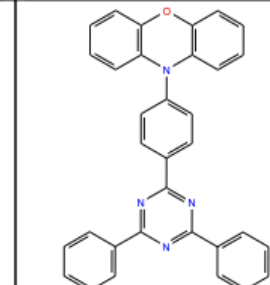
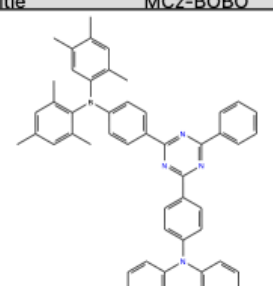
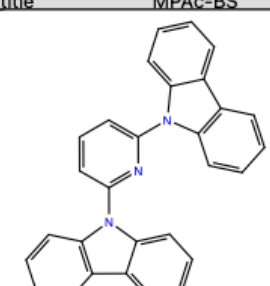
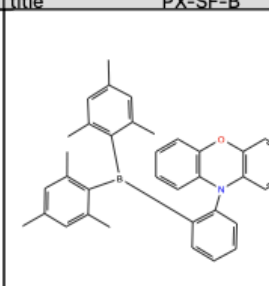
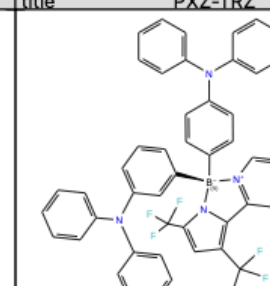
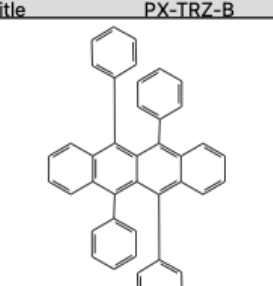
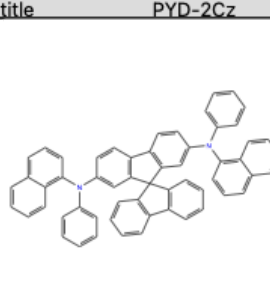
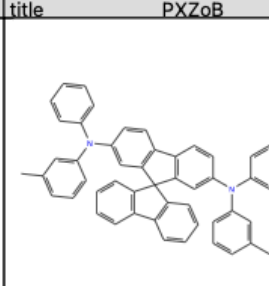
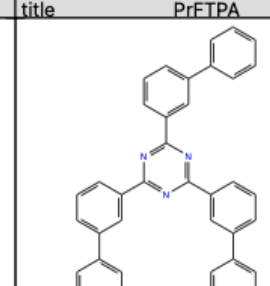
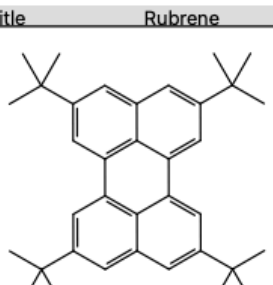
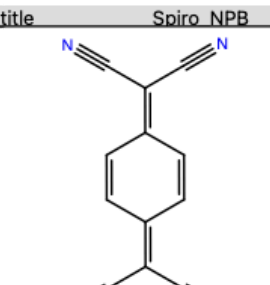
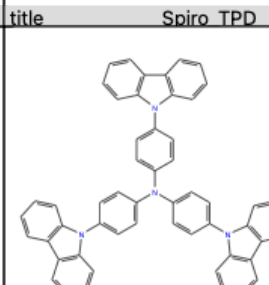
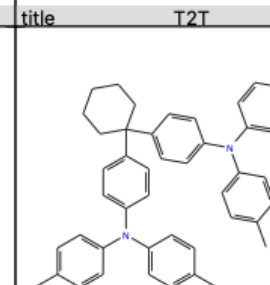
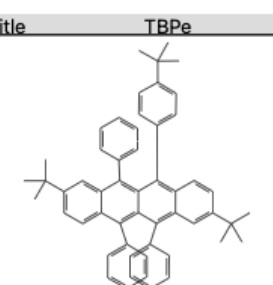
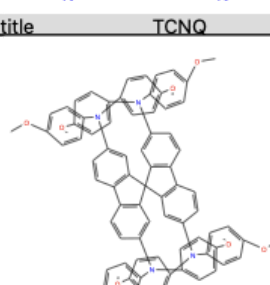
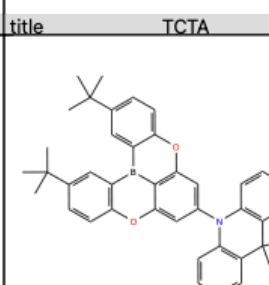
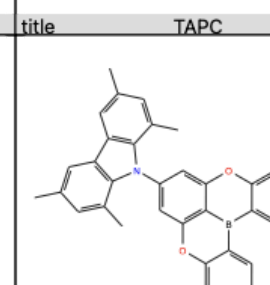
In the supplementary materials, we present:

- (1) Figure S1.** Chemical structure of 100 molecular systems relevant to organic optoelectronics to compare geometry optimization using the MLFF and DFT.
- (2) Table S1.** Benchmarking results (RMSDs and cpu time) for the 100-molecule validation set.

			
title Tris-PCz	title tCP	title TAZ	title PPT
			
title PPO27	title Phen-TRZ	title Pentacene	title p-bPPhenB
			
title oCBP	title DPVBi	title DPPvA	title DMQA
			
title DCz-BTP	title B4PvPPm	title B4PvmPm	title DOBNA-OAr
			
title DiKTa	title DBF-TRZ	title DABNA-1	title BCzPh

			
title 26DCzPPv	title 3TPYMB	title 3DPA2FBN	title 2PTZBN
			
title 3DPA-DiKTa	title 3TPA-DiKTa	title DMAC-BP	title DTAF
			
title 2CzPN	title 3N-T2T	title 3P-T2T	title 2-TNATA
			
title 3DPvMpdTC	title 4CzBN	title 4CzDPO	title 4CzIPN
			
title 4CzPN	title ACRSA	title ADN	title B3PvPB

			
title BPhen	title BTB	title CBP	title BCP
			
title Cz2BP	title DACT-II	title DBP	title DCJTb
			
title DMACDPS	title DMTDac	title DPEPO	title F4TCNQ
			
title HATCN	title MADN	title MPAC-Dip-BS	title NPB
			
title OXD-7	title OBA-BrO	title 4CzPN-tBu	title PAB

			
title MCz-BOBO	title MPAc-BS	title PX-SF-B	title PXZ-TRZ
			
title PX-TRZ-B	title PYD-2Cz	title PXZoB	title PrFTP
			
title Rubrene	title Spiro NPB	title Spiro TPD	title T2T
			
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title TBRb	title Spiro-OMeTAD	title TDBA-AC	title TMCz-BO

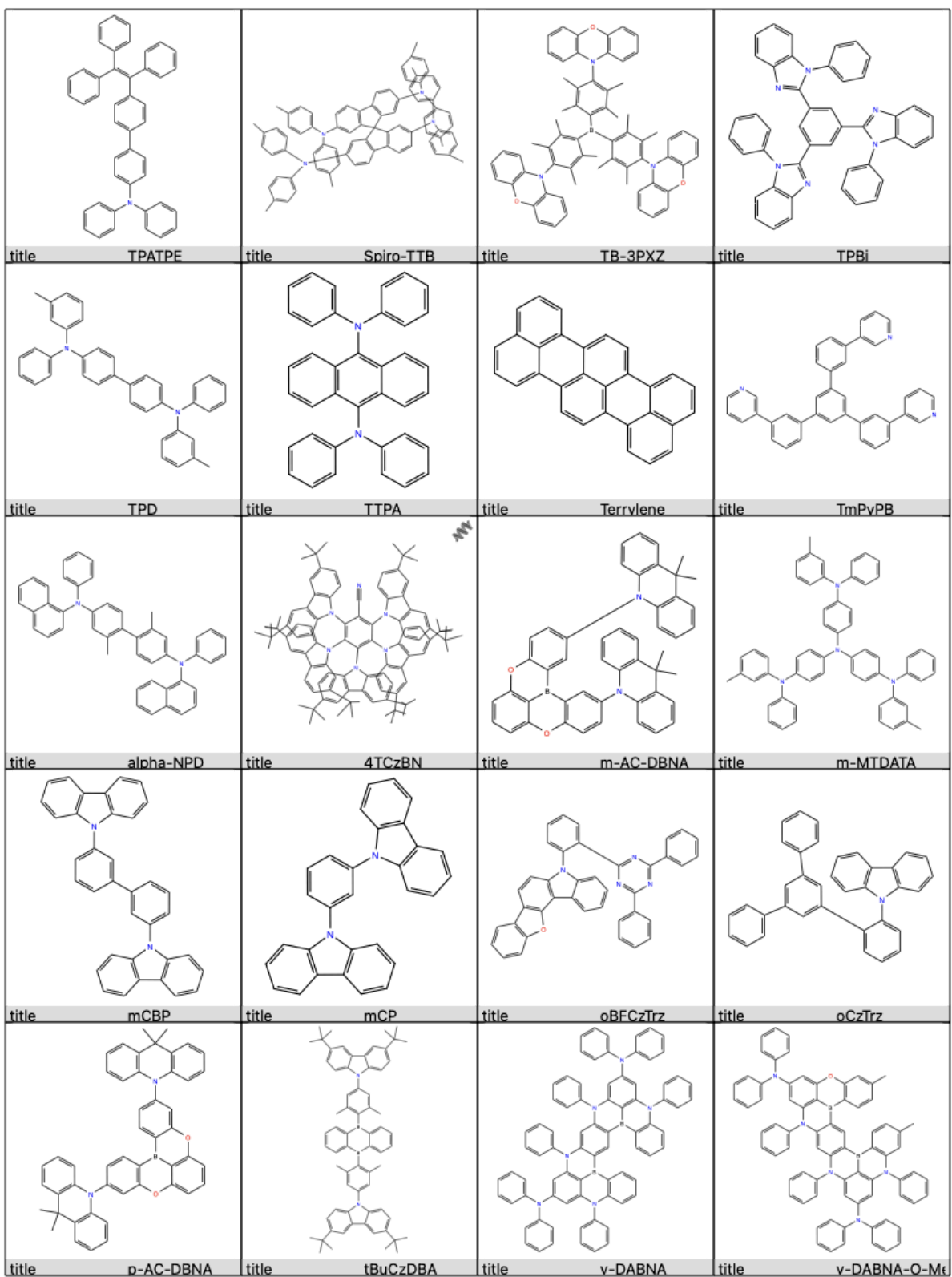


Figure S1. Chemical structure of 100 molecular systems relevant to organic optoelectronics to compare geometry optimization using the MLFF and DFT.

Table S1. Benchmarking results for the 100-molecule validation set. For each molecule (structures provided in Figure S1), the RMSD of atomic positions (including hydrogen atoms) is reported, comparing the final geometry optimized via the MPNICE framework against the DFT reference (B3LYP/6-31G(d,p)). Performance is quantified by the total CPU time (in seconds) required for convergence under identical starting configurations and optimization criteria.

Title	RMSD / Å	MLFF cpu time	DFT cpu time	RMSD per atom / Å
Tris-PCz	0.260	4.725	3711.367	0.003
tCP	0.052	3.758	2254.077	0.001
TAZ	0.209	3.323	3150.639	0.003
PPT	0.419	17.908	31052.131	0.006
PPO27	0.684	4.688	10721.150	0.009
Phen-TRZ	0.064	2.811	6824.624	0.001
Pentacene	0.021	2.362	572.994	0.001
p-bPPhenB	0.598	6.312	16888.264	0.008
oCBP	0.066	7.595	4087.735	0.001
DPVBi	0.234	4.116	6380.640	0.003
DPPyA	0.336	4.415	5530.547	0.005
DMQA	0.020	2.684	452.233	0.000
DCz-BTP	0.100	4.578	5447.432	0.002
B4PyPPm	0.133	4.100	7676.802	0.002
B4PymPm	0.130	3.243	3393.457	0.002
DOBNA-OAr	0.355	9.875	13317.249	0.004
DiKTa	0.054	2.552	1089.796	0.002
DBF-TRZ	0.101	5.068	5650.607	0.001
DABNA-1	0.061	4.373	2165.779	0.001
BCzPh	0.118	3.164	1625.628	0.002
26DCzPPy	0.368	7.534	19009.146	0.005
3TPYMB	0.278	19.664	25056.876	0.003
3DPA2FBN	0.282	11.557	30488.598	0.004
2PTZBN	0.084	4.537	3244.328	0.002
3DPA-DiKTa	0.217	19.979	27339.464	0.002
3TPA-DiKTa	0.718	31.378	80253.361	0.006
DMAC-BP	0.941	5.676	23122.386	0.011
DTAF	0.346	11.098	12443.715	0.003
2CzPN	0.108	5.995	5142.372	0.002
3N-T2T	0.319	3.720	5946.405	0.005
3P-T2T	0.291	3.312	6519.173	0.005
2-TNATA	0.855	23.165	100036.965	0.007

3DPyMpDTC	0.588	9.963	22933.186	0.005
4CzBN	0.290	9.718	26830.289	0.003
4CzDPO	0.265	26.218	86508.804	0.002
4CzIPN	0.082	11.355	8462.507	0.001
4CzPN	0.185	12.858	31381.957	0.002
ACRSA	0.029	3.033	3796.765	0.001
ADN	0.207	3.969	3840.093	0.004
B3PyPB	0.235	3.101	5288.718	0.003
BPhen	0.091	5.053	2845.250	0.002
BTB	0.044	3.760	3411.917	0.001
CBP	0.047	3.247	991.231	0.001
BCP	0.393	5.438	1495.694	0.008
Cz2BP	0.159	3.648	5424.415	0.002
DACT-II	0.565	10.779	50272.718	0.005
DBP	0.053	7.237	12708.602	0.001
DCJTB	0.248	6.757	27996.042	0.004
DMACDPS	0.362	15.108	51812.562	0.004
DMTDAc	0.183	5.205	48508.789	0.002
DPEPO	0.217	5.982	10918.494	0.003
F4TCNQ	0.020	2.739	145.599	0.001
HATCN	0.021	2.865	467.897	0.001
MADN	0.243	4.689	11171.103	0.004
MPAc-Dip-BS	0.245	57.727	96955.623	0.002
NPB	0.602	6.939	18634.899	0.008
OXD-7	0.796	3.005	1001.899	0.012
OBA-BrO	0.281	11.424	28854.298	0.004
4CzPN-tBu	1.327	88.263	307644.715	0.007
PAB	0.262	15.316	14439.709	0.003
MCz-BOBO	0.877	35.297	156827.716	0.006
MPAc-BS	1.660	63.897	97311.691	0.015
PX-SF-B	1.289	8.172	30414.912	0.015
PXZ-TRZ	0.054	3.105	2145.790	0.001
PX-TRZ-B	1.043	11.839	69217.321	0.010
PYD-2Cz	0.047	3.600	2845.653	0.001
PXZoB	0.334	22.514	25023.215	0.005
PrFTPA	0.376	27.128	75664.844	0.004
Rubrene	0.440	6.040	3875.563	0.006
Spiro_NPB	0.633	5.585	55687.524	0.007
Spiro_TPD	0.701	5.511	56863.252	0.008

T2T	0.105	3.483	3249.301	0.002
TBP_e	0.027	3.840	1199.627	0.000
TCNQ	0.022	2.828	113.561	0.001
TCTA	0.171	6.645	37559.444	0.002
TAPC	0.215	12.257	9045.456	0.002
TBR_b	0.413	14.845	30808.046	0.004
Spiro-OMeTAD	0.587	125.526	214406.662	0.004
TDBA-AC	0.194	7.594	17192.408	0.002
TMCz-BO	0.388	7.281	20795.147	0.006
TPATPE	0.116	3.460	19529.953	0.001
Spiro-TTB	0.796	113.566	124045.153	0.005
TB-3PXZ	0.362	50.380	116796.555	0.003
TPBi	0.451	5.893	10017.567	0.006
TPD	0.295	9.924	8547.015	0.004
TTPA	0.094	4.224	6612.787	0.001
Terrylene	0.016	2.418	1355.186	0.000
TmPyPB	0.145	3.331	2613.603	0.002
alpha-NPD	0.311	7.325	35446.901	0.004
4TCzBN	1.403	184.185	485412.687	0.006
m-AC-DBNA	0.761	8.465	68960.941	0.008
m-MTDATA	0.488	23.621	79081.435	0.004
mCBP	0.634	6.845	10228.058	0.010
mCP	0.060	2.875	1149.533	0.001
oBFCzTrz	0.705	5.435	18198.009	0.010
oCzTrz	0.394	3.757	5025.261	0.006
p-AC-DBNA	0.421	8.389	32519.298	0.005
tBuCzDBA	1.644	13.474	116779.175	0.011
v-DABNA	0.871	36.461	122760.083	0.006
v-DABNA-O-Me	0.663	27.045	68222.685	0.005