Supporting Information

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Computational details

Geometry optimization and excited-state property calculations were performed using the M062X/def2SVP level of theory with the Gaussian16 software package. The calculations for excited-state properties included vertical excitation energy calculations based on optimized ground-state structures, geometry optimizations of the S_1 and T_1 states, and single-point energy calculations for the T_1 state. Additionally, we used Multiwfn to calculate the overlap integrals of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) orbitals.

Our approach involves extensive computational chemistry and machine learning tasks. All computational tasks are performed on servers with AMD EPYC™ 7R32 CPUs. The software versions used for computational chemistry are Gaussian 16, Multiwfn 3.7, and Python 3.8. Each TADF molecule's ground state geometry optimization and vertical excitation state calculations require approximately 300 core hours of computational resources. The geometry optimization and single-point energy calculations for the S1 and T1 excited states require approximately 2000 core hours of computational resources. For future researchers, using the M062X/def2SVP method for calculating TADF is sufficient for performing computational chemistry screening.

Machining learning model parameters

The input of the model consists of five types of molecular fingerprints converted from SMILES, including four qualitative molecular fingerprints (Atom-pair, Daylight, Morgan, Topological) and quantitative molecular descriptors (RDKit descriptors). Standardization and Principal Component Analysis (PCA) methods were used to reduce the dimensionality of the features. Initially, the 365 data points were randomly divided into four groups, and the models were trained using grid search and 4-fold cross-validation. Four models, Gradient Boosting Decision Tree (GBDT), Random Forest (RF), K-Nearest Neighbors (KNN), and Extreme Gradient Boosting (XGBoost), were trained. Finally, using all the data for training, the models were integrated using a voting method.

The machine learning model training was conducted using Python 3.8. The training of the ensemble learning model required approximately 7200 core hours of computational resources. For the prediction of Td, researchers can provide us with the TADF molecular structures for the prediction of molecular properties.

Data of 90 molecules selected from 1787 molecules

Table1

Number	$E_{ad}S_1$(eV)	$E_{ad}T_1$(eV)	T_1(eV)	E(RM062X)	$\Delta E_{ad}ST$(eV)	ΔG_{RISC}(eV)
1	2.6319	2.4841	3.0232	-2940.6311	0.1478	0.3659
2	2.4732	2.4026	2.9815	-2479.0407	0.0706	0.3459
3	3.6152	2.4232	3.0462	-2057.1383	1.192	1.1920
4	2.4777	2.5225	3.0586	-3088.5204	-0.0448	0.2965
5	2.8301	2.8255	3.1101	-2075.8658	0.0046	0.1851
6	2.6539	2.5958	3.1062	-2940.6247	0.0581	0.2977
7	2.4761	2.3577	3.233	-2479.0234	0.1184	0.4837
8	2.6665	2.4494	2.9962	-2479.0436	0.2171	0.4153
9	2.5815	2.5633	3.0991	-3510.4325	0.0182	0.3088
10	2.8399	2.848	3.1386	-1909.2266	-0.0081	0.1627
11	2.7804	2.8296	3.1308	-2223.3416	-0.0492	0.1601
12	2.8295	2.5796	3.1302	-2057.1281	0.2499	0.4059
13	3.2682	2.5793	3.085	-2142.4426	0.6889	0.7200
14	2.7414	2.1437	2.9052	-2753.8707	0.5977	0.7792
15	2.5355	1.3988	2.9809	-2135.4443	1.1367	1.4189
16	2.7194	2.6894	3.1491	-2521.8734	0.03	0.2634
17	2.7337	1.7621	3.1727	-2121.5819	0.9716	1.2236
18	3.1615	2.0104	3.2693	-1798.6164	1.1511	1.2565
19	2.8128	2.0128	3.3032	-2034.1987	0.8	1.0188
20	2.8095	2.0143	3.2119	-1948.8668	0.7952	0.9751
21	3.1902	2.4864	3.4232	-2199.3840	0.7038	0.8591
22	3.0315	2.4727	3.5626	-2670.6126	0.5588	0.7836
23	2.9491	2.4018	3.5345	-2818.0963	0.5473	0.7354
24	3.6083	2.71	3.3918	-3852.8594	0.8983	0.9729
25	3.9077	2.9014	3.5404	-2978.5192	1.0063	1.0312
26	2.4627	2.2965	2.985	-2459.1519	0.1662	0.4088
27	2.5034	2.2952	2.9841	-2782.0713	0.2082	0.4329
28	2.1231	2.099	2.7223	-2672.4434	0.0241	0.3060
29	2.5151	2.3031	3.0683	-2154.4057	0.212	0.4442
30	2.5238	2.2515	2.9792	-2154.4117	0.2723	0.4706
31	2.6432	2.2911	3.0464	-2670.1065	0.3521	0.5350
32	2.5924	2.541	2.7921	-2971.5051	0.0514	0.2105
33	2.3101	2.1485	2.8103	-4238.4674	0.1616	0.4891
34	2.5481	2.2372	2.9133	-2254.2180	0.3109	0.4901
35	2.504	2.0726	2.8626	-2168.6877	0.4314	0.5955
36	2.5524	2.0712	2.8893	-2491.6058	0.4812	0.6399
37	2.1452	2.0337	2.6443	-2381.9805	0.1115	0.3385
38	2.5729	2.0582	2.868	-1863.9414	0.5147	0.6484
39	2.6353	2.0366	2.7566	-1863.9442	0.5987	0.6783
40	2.1362	1.6823	2.5421	-2480.1664	0.4539	0.6458
41	2.1936	1.6571	2.5165	-2637.2311	0.5365	0.7067
42	2.0341	1.8337	2.3497	-2173.2466	0.2004	0.3667
43	2.1579	1.6598	2.5293	-3108.3954	0.4981	0.7043
44	2.1014	1.6792	2.4663	-2937.7323	0.4222	0.6024
45	2.7391	1.9611	2.3919	-2483.7492	0.778	0.7929
46	1.9068	0.4973	2.349	-2474.4640	1.4095	1.6129
47	2.3676	1.6374	2.3889	-2954.9115	0.7302	0.8553
48	2.1011	1.8163	2.4439	-2167.4932	0.2848	0.4475
49	2.1553	1.831	2.4243	-2490.4134	0.3243	0.4636
50	2.1119	1.7859	2.4104	-2093.5421	0.326	0.4611
51	2.1481	1.8112	2.4672	-1862.7466	0.3369	0.4803
52	1.9657	1.8142	2.3732	-2378.4423	0.1515	0.3547
53	2.1517	1.7724	2.3574	-1862.7484	0.3793	0.4816
54	2.2551	1.8033	2.4775	-2378.4457	0.4518	0.5703

55	2.2134	1.7829	2.4026	-1694.4515	0.4305	0.5261
56	2.1732	2.0144	2.627	-2103.2229	0.1588	0.4053
57	2.1253	1.6749	2.5374	-1732.5029	0.4504	0.6255
58	2.16	1.6513	2.5116	-1811.0354	0.5087	0.6667
59	2.0753	1.938	2.5648	-2643.9161	0.1373	0.4058
60	2.1282	2.0139	2.5698	-2016.2512	0.1143	0.3503
61	2.0883	1.653	2.5261	-2046.6175	0.4353	0.6320
62	2.071	1.6381	2.4488	-1961.2860	0.4329	0.5990
63	2.1633	1.9274	2.5188	-2534.2874	0.2359	0.4167
64	2.5796	1.9468	2.5838	-3556.8303	0.6328	0.7616
65	2.189	2.0749	2.6041	-3012.7422	0.1141	0.3422
66	2.3617	2.3352	2.7238	-2869.3019	0.0265	0.2873
67	2.4252	2.3593	3.1352	-2389.1900	0.0659	0.4171
68	2.1422	2.1678	2.9747	-3455.0065	-0.0256	0.4091
69	2.2795	2.2424	3.0786	-2654.4863	0.0371	0.4404
70	2.6039	1.598	3.1738	-2418.9160	1.0059	1.3170
71	2.5209	2.5192	3.2327	-3450.3373	0.0017	0.3755
72	2.0251	1.227	2.1257	-3837.0320	0.7981	0.9210
73	2.5609	2.1218	2.9162	-2527.6197	0.4391	0.6137
74	2.3801	2.2213	2.9471	-2127.3482	0.1588	0.4093
75	2.7132	2.1365	3.2155	-2134.0164	0.5767	0.8015
76	2.7646	2.3155	3.0705	-1923.0871	0.4491	0.5936
77	2.8043	2.3225	3.1067	-2246.0051	0.4818	0.6275
78	2.4462	2.2504	2.8839	-2136.3790	0.1958	0.3927
79	2.1422	2.1679	2.9747	-3455.0065	-0.0257	0.4089
80	2.7445	2.1778	3.0332	-1999.3593	0.5667	0.6756
81	2.6039	1.5905	3.1738	-2418.9157	1.0134	1.3253
82	2.4642	1.929	2.9087	-2231.2109	0.5352	0.7633
83	2.4597	1.9063	2.9186	-2554.1285	0.5534	0.7913
84	2.416	2.1145	2.7974	-2444.5105	0.3015	0.4885
85	2.7439	2.6046	3.1989	-2388.0814	0.1393	0.3807
86	2.7226	2.3292	3.4171	-2271.9822	0.3934	0.6911
87	2.7096	2.4204	3.0951	-2361.9962	0.2892	0.4986
88	2.9487	2.5001	3.2082	-2877.7184	0.4486	0.6208
89	3.1201	2.4975	3.2165	-2228.1833	0.6226	0.7514
90	2.5399	2.6905	3.1407	-2559.1115	-0.1506	0.1689

Table2

Number	Angel (°)	$K_F(s^{-1})$
1	62	8853806.97
2	61	16568157.94
3	55	1190576.80
4	48	13638642.39
5	56	133208.87
6	57	433811.65
7	54	3788722.10
8	51	16972426.63
9	58	2482629.87
10	57	530901.76
11	57	1593236.82
12	59	2650746.02
13	49	59745.75
14	75	21744243.13
15	85	0
16	50	2995441.77
17	80	10292308.85
18	53	1383253.67

19	55	895976.30
20	54	661893.59
21	70	59745.75
22	48	245842.01
23	50	1037296.04
24	48	58849.71
25	45	656402.14
26	43	131600.86
27	41	12181843.08
28	46	3675031.71
29		81631.09
30	35	20283406.06
31	47	2931234.56
32	49	1598921.31
33	61	13088921.29
34	74	8953939.72
35	68	1622033.08
36	70	3121360.57
37	48	4065097.39
38	67	7172832.41
39	49	20676806.12
40	34	4442209.26
41	34	76574.13
42	88	71006931.98
43	34	2251117.19
44	34	7594880.35
45	54	199013.05
46	58	979866.65
47	54	0
48	48	4014685.35
49	51	172370.43
50	59	39942.13
51	49	9268199.45
52	46	224651.81
53	55	19525051.25
54	56	5201167.74
55	59	8733268.41
56	51	4491502.61
57	66	3504783.53
58	65	7668724.05
59	44	3390175.83
60	46	4408085.54
61	65	13606376.12
62	67	519830.63
63	64	667034.70
64	72	661893.59
65	53	47975918.47
66	63	798221.30
67	73	29165.52
68	49	97808.50
69	86	0
70	46	732831.11
71	51	76156143.80
72	54	3759153.04
73	55	4480158.15
74	70	54904.28
75	64	375411.29

76	68	1916229.81
77	70	6409939.55
78	49	3629294.70
79	49	380762.55
80	38	20309.50
81	45	10414440.86
82	68	38335783.43
83	70	734779.70
84	49	15883670.63
85	69	34406379.54
86	61	13391927.43
87	89	347135.21
88	79	6824809.61
89	68	58849.71
90	49	62844910.73