SUPPORTING INFORMATION

1. Effect of the exchange-correlation functional and the solvent on the calculated absorption spectra.

DYE	Exp.[1]	This work		Stein[2]	Kurashige[3]			Wong[4]
		PBE 6-31G (d,p)	B3LYP 6-31G (d,p)	BNL 6-31+G (d,p)	CC2	CIS	B3LYP 6-31+G (d,p)	LC-BLYP 6-31+G (d,p)
C343	2.81	3.00	3.40	3.4	3.44	4.40	3.32	3.36
NKX-2311	2.46	2.35	2.63	2.6	2.71	3.50	2.56	2.73
NKX-2586	2.45	2.15	2.45	2.5	2.66	3.34	2.40	2.66

Table 1. Experimental and computed maximum absorption band energies (eV) for free C343, NKX-2311 and NKX-2586.

[1] K. Hara, T. Sato, R. Katoh, A. Furube, Y. Ohga, A. Shinpo, S. Suga, K. Sayama, H. Sugihara, and H. Arakawa, *J. Phys. Chem. B,* 2003, **107**, 597.

[2] Stein, T.; Kronik, L.; Baer, R. *J. Chem. Phys.* **2009**, *131*, 244119.

[3] Kurashige, Y.; Nakajima, T.; Kurashige, S.; Hirao, K. *J. Phys. Chem. A* **2007**, *111*, 5544.

[4] Wong, B. M.; Cordaro, J. G. *J. Chem. Phys.* **2008**, *129*, 21403.
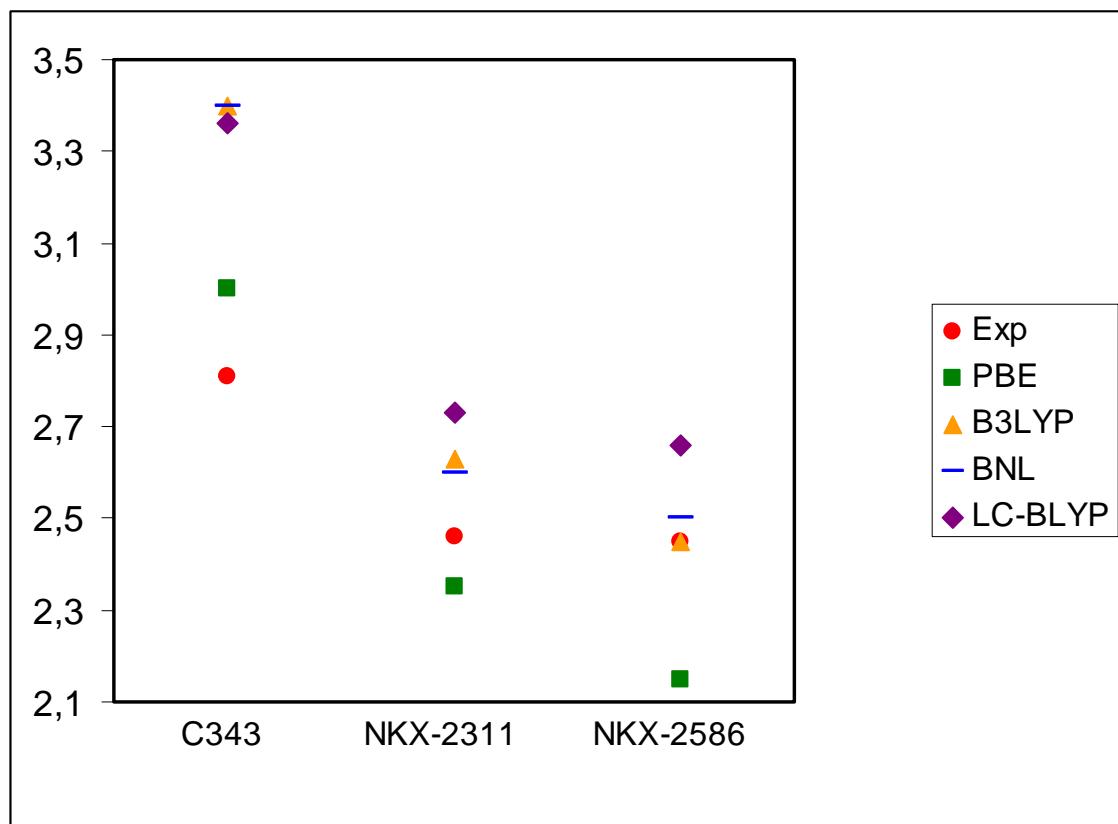
Figure 1. Experimental (Hara) and computed maximum absorption band energies (eV) for free C343, NKX-2311 and NKX-2586. TD-DFT excitation energies calculated with different exchange-correlation functionals are compared: PBE (this work), B3LYP (this work), BNL (Stein) and LC-BLYP (Wong).

Dye	B3LYP (Gas phase)	B3LYP (Methanol)	PBE (Gas phase)	PBE (Methanol)
C343	3.40	3.15	3.00	2.82
NKX-2311	2.63	2.42	2.35	2.18
NKX-2586	2.45	2.20	2.15	1.95

Table 2. Maximum absorption band energies (eV) for free C343, NKX-2311 and NKX-2586 calculated with and without solvent effects (Methanol, PCM).

In figure 1 and table 1 the maximum absorption energies calculated with different methods have been compared for three free dyes: C343, NKK-2311 and NKX-2586. Experimental energies have been also included. In this work we have done PBE and B3LYP calculations for these three free dyes using 6-31G (d,p) basis set. PBE provides better results than B3LYP for C343 and NKX-2311 while B3LYP works better when the molecule size increases (NKX-2586). For these molecules the inclusion of long range corrections in the functional (LC-BLYP or BNL vs. B3LYP) has a very little influence on the results and in the case of NKX-2586 results obtained with these corrected functionals are even worse than B3LYP results. The inclusion of an additional diffuse base functions (B3LYP/6-31G (d,p).vs. B3LYP/6-31+G (d,p)) also has a little effect on the results (less than 0.08 eV) at a considerable computational effort. As it has been said before, CIS method always overestimates the excitation energies and CC2 provide, for the studied molecules, results similar to B3LYP, but with a much more computational effort. There is not previously published data about calculations on NKX-2753 and NKX-2593. Nevertheless, these molecules have a similar size to NKX-2586 and might share the same technical shortcomings.

We can conclude that, although as a general statement the use of long range corrected B3LYP and an additional diffuse base functions might be a better choice for dye molecules, for these particular dyes they do not improve substantially the results. This is a consequence of the kind of excitation we are dealing with. Since this kind of molecules work on an indirect mechanism (intramolecular excitation followed by a charge transfer to the conduction band of the semiconductor), the charge transfer character of the excitation is moderate.

We have also done preliminary calculations in order to estimate the effect of the inclusion of a solvent on the absorption spectra of free dyes. We have done the frequency domain TD-DFT calculations for the free dyes using PBE and B3LYP and with and without methanol solvent effects (PCM model). Results are shown in Table 2. In all cases, the inclusion of solvent effects red shifts the first transition about 0.15-0.20 eV, but that does not improve necessarily the result with respect to the experimental values as can be seen from Table 2. Even considering the solvent effects, PBE reproduces better C343 experimental spectrum, while B3LYP with solvent effects reproduces better NKX-2311 and NKX-2586 experimental data.

2. Study of the different bidentate adsorption modes and its influence on the electronic absorption spectra.

bb   **bc**
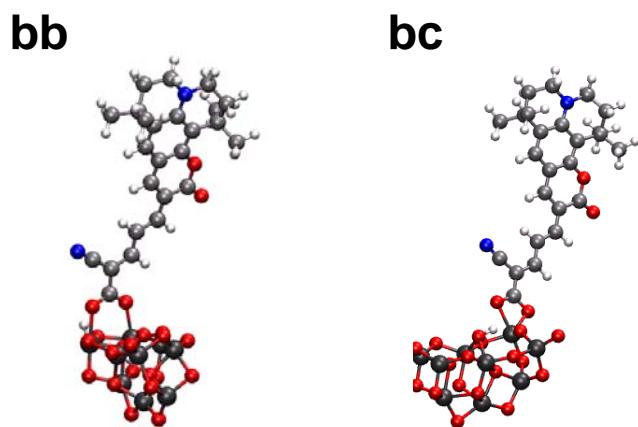
Figure 2. Two bidentate adsorption modes for NKX-2311 on $(TiO_2)_9$ are possible: bidentate bridging (bb) structure with both dye oxygen atoms bound to two cluster titanium atoms or a bidentate structure with the two dye oxygens bound to the same cluster titanium atom, in a chelating configuration (bc). For all considered dyes the most stable adsorption mode is the bidentate chelating configuration (bc), with the dissociated hydrogen bound to an oxygen in the centre of the cluster.
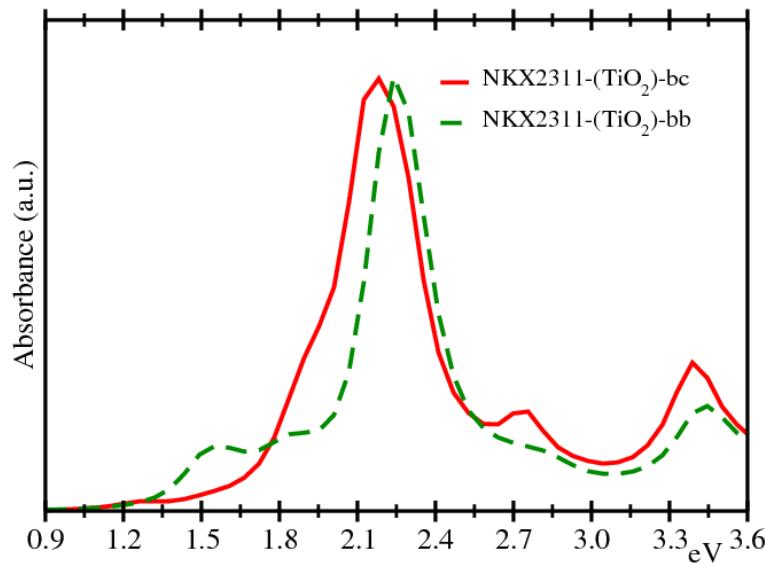
Figure 3. RT-TDDFT spectra for adsorbed NKX-2311 in its two possible bidentate adsorption modes (bb and bc). The absorption maximum position in the spectra is almost not affected by the adsorption mode (differences less than 0.07 eV). Nevertheless, for the bidentate bridging structure (bb) a new band at lower energy appears in the simulated spectrum, which is not present in the experimental spectrum.

3. Geometric data

Optimized geometries for free and adsorbed dyes

FREE C343

C	0.227180	-5.949616	-0.115580
C	-1.158575	-5.911512	-0.111791
C	-1.131332	-3.480363	0.024342
C	-0.854669	-0.977913	0.199701
C	0.924395	-7.273963	-0.163899
C	0.976407	-4.716416	-0.076338
C	-1.871455	-4.689596	-0.055624
C	-1.717589	-2.216849	0.111441
C	-1.638366	0.273776	-0.199051
C	-3.285138	-4.575848	-0.077686
C	-3.144614	-2.144645	0.104163
C	-2.998544	0.291842	0.495749
C	-3.928656	-3.349761	-0.002514
C	-5.440249	-3.272507	-0.019293
C	-5.229251	-0.793431	0.222381
C	-5.910816	-1.918221	-0.552576
N	-3.769646	-0.914915	0.184693
O	0.306077	-8.340618	-0.199905
O	0.253778	-3.522363	0.012576
O	2.216882	-4.598730	-0.111905
O	2.279912	-7.234901	-0.156013
H	-0.464944	-0.872576	1.224376
H	0.030795	-1.103567	-0.436225
H	-1.790631	0.293524	-1.286274
H	-1.687238	-6.865627	-0.153314
H	-1.079994	1.179694	0.067339
H	2.580431	-6.271754	-0.142170
H	-3.589501	1.155245	0.161564
H	-2.872495	0.389515	1.588294
H	-3.878927	-5.487913	-0.158440
H	-5.490422	0.181304	-0.213831
H	-5.843268	-4.092590	-0.628570
H	-5.833629	-3.425366	0.998109
H	-5.584164	-0.778991	1.267812
H	-5.664626	-1.828868	-1.619543
H	-6.999180	-1.816151	-0.455973

ADSORBED C343

Ti	15.618100	4.915257	15.538679
Ti	14.656039	6.531828	13.342110
Ti	17.613459	6.270851	13.085940
Ti	14.907321	7.679475	15.895440
Ti	20.753710	6.862666	12.242809
Ti	18.144937	4.270597	15.519405
Ti	20.762607	5.138394	14.770070
Ti	17.901846	7.483138	15.838273
Ti	21.136004	8.061333	15.539596
O	14.320878	4.940144	14.100751
O	16.506931	3.427434	16.089748
O	15.998929	6.523090	12.119939
O	16.415538	8.474763	16.506535
O	13.865553	7.895651	14.349067
O	14.579851	6.088665	16.664016
O	21.360157	5.298375	13.036662
O	17.128385	4.584195	13.950862
O	19.874559	3.641029	15.478823
O	19.052090	5.949794	14.729390
O	21.668387	6.233360	15.834641
O	18.970420	6.233881	11.961490
O	17.978321	8.085584	13.904925
O	20.702593	8.038422	13.605830
O	17.393451	5.716852	16.531218
O	22.237354	9.179450	15.984697
O	19.397398	8.197210	16.403101
O	16.051565	6.719305	14.671194
O	21.750064	10.977763	7.818746
O	19.928599	10.149762	8.841768
O	20.292882	8.046682	10.580991
O	22.342746	7.399126	11.052910
C	22.067730	9.112799	9.350390
C	23.427587	9.141071	9.049714
C	23.092096	11.006084	7.525572
C	21.138093	10.044007	8.713744
C	23.971206	10.061655	8.127870
C	23.524496	11.996380	6.642917
C	23.050500	13.441947	4.673815
C	25.343916	10.127230	7.764021
C	24.908797	12.030098	6.299949
C	24.484347	13.951917	4.769786
C	25.820627	11.060460	6.859301
C	26.801607	13.165466	5.128406
C	21.550694	8.168354	10.328011
C	27.704315	12.549258	6.192021
C	27.275359	11.102406	6.453262
C	22.558322	12.994883	6.051995
N	25.376016	12.990785	5.432200

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H	27.019301	12.725618	4.139700
H	27.634504	13.131832	7.120368
H	28.745212	12.601285	5.849709
H	18.931330	8.328481	13.694503
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H	22.464664	13.866216	6.719984
H	21.557842	12.551774	5.993305
H	27.894906	10.639793	7.232625
H	27.428024	10.506762	5.538499

FREE NKX-2311

C	0.271203	-0.799692	1.319622
C	-0.382158	-0.170734	-1.033264
C	0.573109	-5.620532	-0.406409
C	-0.821298	-5.651878	-0.360889
C	-0.970483	-3.228023	-0.100436
C	-0.906386	-0.695948	0.321566
C	1.414466	-6.786300	-0.475240
C	1.243943	-4.321339	-0.350700
C	-1.611074	-4.491130	-0.217897
C	-1.655401	-2.024778	0.116067
C	-1.880480	0.323688	0.945618
C	0.994525	-8.100303	-0.518400
C	-3.026577	-4.515552	-0.161974
C	-3.096994	-2.091508	0.098929
C	-3.213067	0.383169	0.228719
C	1.914165	-9.181750	-0.513538
C	-3.782362	-3.365300	-0.023101
C	1.577523	-10.529001	-0.538739
C	-5.311101	-3.443743	0.018643
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C	0.214358	-10.936581	-0.587914
C	2.665818	-11.524469	-0.506336
C	-5.857172	-4.618485	-0.814042
C	-5.780598	-3.606190	1.481904
C	-5.861753	-2.140612	-0.589024
N	-3.841553	-0.935491	0.189131
N	-0.938831	-11.195155	-0.626877
O	0.405972	-3.184853	-0.218900
O	2.451681	-4.102047	-0.410356
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O	3.871363	-11.261825	-0.438670
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H	-1.412886	1.317874	0.937381
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H	-1.334724	-6.613550	-0.418607
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H	-3.518011	-5.484071	-0.249491
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H     2.996792  -13.398743   -0.539407
H    -5.724635   -0.814186    1.125032
H    -5.600085   -2.103417   -1.656205
H    -6.958337   -2.127888   -0.522058
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ADSORBED NKX-2311

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Ti   23.099910    2.616704   12.032520
Ti   23.071512   -1.868490   14.041095
Ti   21.504688    0.081693   12.658739
Ti   24.618396   -1.631053   11.211204
Ti   22.256619    0.103610    9.702259
O    27.013934   -2.131507   15.262237
O    23.893041   -3.227080   15.133777
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O    28.664672   -1.999707   12.759905
O    26.520335   -4.055202   13.253078
O    21.625512    1.908308   12.901178
O    24.551369   -0.857742   14.669449
O    21.353423   -1.210832   14.013333
O    23.314689   -0.457480   12.547092
O    20.908246   -0.274440   11.026995
O    24.351235    1.986986   13.330465
O    25.438021    0.214435   11.352540
O    23.205363    1.621904   10.541952
O    24.040912   -2.800932   12.674773
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C	28.868927	11.610299	3.964729
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N	26.494876	14.370549	4.093482
N	26.880030	6.311819	10.160448
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H	22.871068	14.835944	6.688284
H	22.591980	12.477910	3.785810
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H	23.460711	15.535482	3.096538
H	24.125525	15.894883	6.018897
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H	24.189733	13.982140	2.670440
H	22.410173	6.972974	10.479596
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H	28.219523	11.785700	3.097567
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H	28.688271	10.581398	4.300491
H	28.005740	13.988653	2.675065
H	28.840527	14.716378	5.538404
H	29.892851	14.121389	4.246801
H	30.590549	12.486745	5.971183
H	29.914705	11.680514	3.632060
H	24.838913	0.858357	10.873311
H	27.472082	10.874071	6.883180

FREE NKX-2586

C	0.258009	-0.783343	1.316085
C	-0.395030	-0.134919	-1.033798
C	0.565189	-5.617344	-0.396782
C	-0.829065	-5.635113	-0.354888
C	-0.918100	-0.669448	0.317720
C	-0.974653	-3.207447	-0.115221
C	1.236822	-4.316350	-0.358577
C	1.396005	-6.793944	-0.479825
C	-1.615983	-4.470098	-0.225371
C	-1.661008	-2.002970	0.103731
C	-1.896312	0.343208	0.949362
C	0.961315	-8.105676	-0.495841
C	-3.030219	-4.495367	-0.170667
C	-3.103017	-2.072290	0.091825
C	-3.230795	0.402292	0.233759
C	1.832518	-9.227125	-0.588083
C	-3.786117	-3.346323	-0.029159
C	1.395796	-10.543661	-0.610923
C	-5.312938	-3.429898	0.029897
C	-5.316083	-0.899402	0.105550
C	2.280794	-11.648061	-0.717550
C	-5.759367	-3.589171	1.499975
C	-5.868034	-4.610413	-0.786773
C	-5.874356	-2.133601	-0.579647
C	1.911982	-12.990089	-0.745950
C	0.539656	-13.372100	-0.667470
C	2.896051	-14.081404	-0.853338
O	0.401138	-3.173370	-0.241501
O	2.442982	-4.093430	-0.423322
O	4.194619	-13.621171	-0.973439
O	2.638680	-15.287984	-0.841945
N	-3.853529	-0.918756	0.187499
N	-0.615172	-13.619260	-0.607643
H	-0.060575	-1.276692	2.243618
H	0.119763	0.825519	-0.889190
H	0.319590	-0.837149	-1.477887
H	0.600501	0.227865	1.576764
H	2.470401	-6.602786	-0.526628
H	1.108501	-1.333269	0.909168
H	-1.206977	0.018686	-1.756911
H	-1.353927	-6.590182	-0.408778
H	-1.433557	1.340275	0.949377
H	-2.072589	0.069371	1.999993
H	2.907385	-9.032107	-0.647606
H	-3.122959	0.800274	-0.790798
H	-0.107631	-8.330191	-0.438074
H	-3.524269	-5.462402	-0.255182
H	-3.918060	1.075125	0.765486

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H    -5.371241   -2.790117   2.144036
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H    -5.598346   -5.581112  -0.353421
H    -5.622555   -2.102609  -1.649155
H    -5.602665    0.001699  -0.455852
H    -5.737452   -0.787117   1.119126
H    -6.855602   -3.588995   1.573440
H    -6.964668   -4.561762  -0.804348
H    -6.970069   -2.123033  -0.502773
H     4.760374  -14.422958  -1.029996
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ADSORBED NKX-2586

Ti	24.839354	-10.226695	3.369548
Ti	22.090926	-9.847206	2.610665
Ti	23.509203	-7.216088	2.338617
Ti	22.755606	-10.005095	5.336307
Ti	24.191823	-3.984331	2.052903
Ti	26.477274	-8.227896	3.080660
Ti	26.701139	-5.391370	3.156398
Ti	24.256274	-7.381682	5.261056
Ti	25.145861	-4.198912	5.483091
O	23.461294	-10.923155	2.200658
O	26.594620	-10.143110	2.920348
O	22.082571	-8.268365	1.687053
O	23.206464	-8.566523	6.337916
O	21.300367	-10.394630	4.213190
O	24.130593	-11.090454	4.936523
O	26.001222	-4.380009	1.830305
O	24.941907	-8.493196	1.971310
O	27.731356	-6.924750	2.807723
O	25.273251	-6.600928	3.504825
O	26.867464	-4.486686	4.678757
O	23.477064	-5.629451	1.491365
O	22.819930	-6.514516	4.099780
O	24.039793	-3.999789	3.857064
O	25.624519	-8.700238	4.726375
O	25.044376	-2.974087	6.557599
O	24.712824	-5.973367	6.185218
O	23.303347	-8.946428	3.810883
O	16.986116	7.246202	1.406151
O	16.728097	5.332320	2.551798
O	22.646071	-2.581238	1.731557
O	24.648124	-2.349455	0.850513
C	14.579170	8.459546	0.503410
C	15.620130	10.051591	2.159374
C	18.708636	5.520303	1.179962
C	19.395669	6.412223	0.352695
C	15.577818	9.629455	0.673980
C	17.627492	8.088807	0.520367
C	17.441439	5.957182	1.770383
C	19.134194	4.181667	1.492662
C	18.894842	7.688618	0.015847
C	16.997445	9.293321	0.180698
C	15.021885	10.776066	-0.194931
C	20.264174	3.540502	1.021253
C	19.573951	8.596713	-0.836362
C	17.760096	10.214348	-0.627103
C	15.992403	11.930464	-0.340076
C	20.584779	2.191283	1.329953
C	19.055775	9.837667	-1.162060

C	21.709898	1.542216	0.839632
C	19.821418	10.787410	-2.087830
C	18.017847	12.500347	-1.616853
C	22.030063	0.194458	1.124760
C	19.367156	10.563965	-3.548153
C	21.345229	10.585291	-2.010568
C	19.511221	12.225615	-1.632072
C	23.183834	-0.454071	0.682561
C	24.151803	0.227951	-0.113188
C	23.481166	-1.822000	1.080982
N	17.266365	11.473194	-0.891710
N	24.907834	0.845317	-0.779647
H	14.621618	8.048993	-0.513976
H	14.611215	10.315147	2.507228
H	15.988588	9.230075	2.784199
H	13.560394	8.838024	0.667892
H	18.464199	3.632055	2.157223
H	14.753090	7.646265	1.210667
H	16.275303	10.917023	2.324177
H	20.355733	6.116393	-0.075581
H	14.082612	11.138623	0.244248
H	14.781286	10.388842	-1.196075
H	19.901277	1.639574	1.981661
H	16.165910	12.434897	0.626222
H	20.955760	4.067747	0.358593
H	20.542922	8.292882	-1.230080
H	15.585826	12.687531	-1.025247
H	21.356122	-0.396189	1.749296
H	18.282006	10.668696	-3.670099
H	21.710662	10.657479	-0.978044
H	19.633810	9.551878	-3.877200
H	22.398070	2.102031	0.201055
H	21.658756	9.616236	-2.418376
H	19.923721	12.379310	-0.624227
H	17.817367	13.463739	-1.126187
H	17.621849	12.584227	-2.642923
H	19.859132	11.281161	-4.220996
H	21.850435	11.358678	-2.604520
H	20.002187	12.948795	-2.298217
H	22.985087	-5.524506	4.096735

FREE NKX-2753

C	0.318245	-0.909251	1.337920
C	-0.355467	-0.242641	-0.996392
C	0.346661	-5.768577	-0.465799
C	-1.042526	-5.717873	-0.378614
C	-0.873858	-0.757166	0.364263
C	-1.049809	-3.297694	-0.040102
C	1.093968	-4.514855	-0.351354
C	1.111174	-6.978111	-0.672014
C	-1.762056	-4.519738	-0.172595
C	-1.673465	-2.057098	0.170258
C	-1.806147	0.289293	1.010311
C	2.842589	-9.451115	-1.085577
C	3.177930	-10.327655	-3.425381
C	4.938709	-10.697854	-1.680607
C	0.588320	-8.241982	-0.836510
C	3.426177	-10.600271	-1.930791
C	-3.174836	-4.475721	-0.077340
C	-3.114764	-2.050639	0.154721
C	-3.132265	0.428201	0.290477
C	1.333914	-9.447860	-1.062867
C	-3.862726	-3.288750	0.093936
C	2.763030	-11.932486	-1.512421
C	0.634879	-10.633249	-1.259438
C	-5.382991	-3.259460	0.237309
C	-5.257032	-0.749894	-0.028821
C	1.249887	-11.900371	-1.516542
C	-5.748565	-3.129199	1.734116
C	-6.057621	-4.518695	-0.328491
C	-5.876467	-2.034197	-0.557366
C	0.439078	-13.036596	-1.703352
C	-0.982581	-12.878085	-1.605194
C	0.824433	-14.436783	-1.966386
O	0.327730	-3.336781	-0.150317
O	2.312638	-4.360361	-0.416056
O	2.166755	-14.664642	-2.216241
O	0.024370	-15.379353	-1.982875
N	-3.812437	-0.860086	0.200332
N	-2.145084	-12.676498	-1.523559
H	0.013008	-1.415232	2.263127
H	0.201683	0.695296	-0.858680
H	0.320718	-0.973089	-1.455340
H	0.682017	0.092049	1.608857
H	2.192198	-6.831964	-0.703873
H	1.150552	-1.465540	0.902348
H	-1.173172	-0.053776	-1.704085
H	-1.617441	-6.641392	-0.471012
H	3.679465	-9.400708	-3.734834
H	5.443455	-9.766133	-1.972146

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H    -1.296071    1.261641    1.027694
H     3.225892   -8.489638   -1.456985
H     3.201903   -9.536632   -0.045421
H    -1.995733    0.006241    2.056085
H     5.160273  -10.884687   -0.619953
H     2.109726  -10.222019   -3.650676
H     3.571826  -11.146170   -4.042057
H     5.380518  -11.514694   -2.267099
H    -2.999192    0.854145   -0.719472
H    -0.497635   -8.373583   -0.807445
H    -3.719534   -5.416166   -0.150545
H     3.139233  -12.744796   -2.139333
H    -3.794134    1.117618    0.836344
H    -5.245967   -2.279317    2.212645
H     3.080237  -12.179616   -0.483442
H    -5.782347   -4.688446   -1.377433
H    -5.444568   -4.033148    2.276453
H    -0.455659  -10.593055   -1.226914
H    -5.797830   -5.418424    0.244280
H    -5.617841   -2.170098   -1.61768
H    -5.420942    0.070564   -0.745538
H    -5.743976   -0.442067    0.912485
H    -6.833136   -3.003188    1.862831
H    -7.148843   -4.411143   -0.277516
H    -6.971001   -1.951749   -0.500376
H     2.237520  -15.635169   -2.363627
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ADSORBED NKX-2753

Ti	-3.804584	-11.843428	6.366145
Ti	-4.518442	-10.382530	3.970664
Ti	-1.600285	-10.968422	3.903983
Ti	-4.252364	-8.993487	6.400144
Ti	1.599136	-10.829912	3.201809
Ti	-1.363803	-12.741298	6.569395
Ti	1.363245	-12.207700	5.914257
Ti	-1.271937	-9.501564	6.530804
Ti	2.027431	-9.283177	6.383054
O	-5.038453	-11.841570	4.869633
O	-3.111336	-13.348278	7.114618
O	-3.120802	-10.671833	2.830344
O	-2.687921	-8.306225	7.001895
O	-5.210465	-8.854711	4.786871
O	-4.773914	-10.454799	7.300061
O	2.028449	-12.338775	4.210085
O	-2.270914	-12.497026	4.910142
O	0.289760	-13.516661	6.738498
O	-0.262822	-11.261152	5.651657
O	2.333943	-11.110651	6.913558
O	-0.197315	-11.248742	2.839151
O	-1.052179	-9.129155	4.550667
O	1.695350	-9.540607	4.465583
O	-2.006475	-11.121078	7.370323
O	3.225958	-8.242782	6.761101
O	0.256048	-8.874069	7.102097
O	-3.160424	-10.186815	5.333757
O	6.889528	-8.646620	-9.105954
O	6.914322	-10.691945	-8.168150
O	2.922791	-11.038184	1.664105
O	1.526767	-9.329551	1.686090
C	9.017446	-7.974174	-10.904521
C	6.890496	-8.113923	-12.255796
C	5.937837	-8.912290	-6.864448
C	5.635845	-7.550606	-6.905703
C	7.786429	-7.183991	-11.409200
C	6.608197	-7.293149	-9.128197
C	6.593988	-9.513687	-8.023486
C	5.643497	-9.782116	-5.751251
C	5.942726	-6.726514	-8.008151
C	6.976154	-6.556283	-10.262404
C	8.350824	-6.043386	-12.280945
C	5.051820	-11.646411	-3.340731
C	2.753786	-12.621722	-2.913855
C	4.791924	-13.800331	-2.064759
C	4.996495	-9.389111	-4.601233
C	4.167885	-12.423157	-2.336521
C	5.634397	-5.342553	-8.051381

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C    6.528090   -5.187299  -10.312060
C    7.302253   -5.015803  -12.659688
C    4.680823  -10.188248   -3.457217
C    5.909204   -4.562323   -9.159077
C    4.099175  -11.633943   -1.005370
C    4.010584   -9.561301   -2.412460
C    5.586636   -3.068096   -9.192033
C    6.078696   -3.128449  -11.673090
C    3.654631  -10.204071   -1.195684
C    6.870363   -2.256224   -8.903017
C    4.509616   -2.664163   -8.171880
C    5.056824   -2.765814  -10.607393
C    2.891634   -9.494099   -0.251071
C    2.419599   -8.182423   -0.577584
C    2.446443   -9.966871    1.047497
N    6.678576   -4.449736  -11.466045
N    2.059398   -7.103376   -0.899507
H    9.608739   -7.373075  -10.201043
H    7.471216   -8.547785  -13.082130
H    6.501111   -8.937878  -11.647306
H    9.661391   -8.215063  -11.761938
H    5.973275  -10.814904   -5.871711
H    8.745703   -8.910916  -10.413228
H    6.032299   -7.579864  -12.684694
H    5.142371   -7.081915   -6.052510
H    2.793453  -13.215749   -3.837524
H    4.868011  -14.385722   -2.991575
H    8.796599   -6.469536  -13.190031
H    5.008844  -12.133444   -4.326390
H    6.106981  -11.709326   -3.021326
H    9.158412   -5.536384  -11.732778
H    5.800504  -13.709736   -1.638147
H    2.263797  -11.669091   -3.149441
H    2.115890  -13.158378   -2.198660
H    4.177881  -14.375217   -1.358219
H    6.527940   -5.451040  -13.315203
H    4.674521   -8.347367   -4.518041
H    5.154185   -4.902126   -7.178323
H    3.452505  -12.150535   -0.287642
H    7.761279   -4.187207  -13.218599
H    7.695179   -2.528912   -9.572956
H    5.100455  -11.621400   -0.540850
H    3.587449   -3.245613   -8.301771
H    7.212153   -2.438569   -7.876833
H    3.735679   -8.511656   -2.534757
H    4.851420   -2.789297   -7.136247
H    4.128685   -3.332649  -10.768325
H    5.602091   -3.131898  -12.665324
H    6.882855   -2.374470  -11.716018
H    6.680787   -1.178457   -9.012695
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H     4.261201  -1.601830  -8.299495
H     4.805952  -1.700519 -10.704203
H    -0.071324  -9.006076   4.370371
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FREE NKX-2593

C	-0.101647	-0.249980	1.415086
C	0.179919	-5.070605	-0.350551
C	0.718386	-7.548542	-0.477564
C	-0.706169	0.402697	-0.943603
C	1.102087	-13.394569	-0.705460
C	0.852477	-3.769298	-0.305584
C	1.053603	-6.214947	-0.456003
C	-1.212631	-5.093455	-0.297394
C	-1.258681	-0.129078	0.396442
C	-1.346012	-2.664931	-0.030014
C	1.691612	-8.601423	-0.571206
C	-1.996096	-3.921552	-0.153020
C	-2.019272	-1.450961	0.176026
C	-2.232687	0.896145	1.011365
C	2.522317	-13.390470	-0.793951
C	2.837062	-10.858766	-0.714865
C	3.095461	-8.515265	-0.651808
C	3.257449	-12.211440	-0.793277
C	3.156644	-14.716311	-0.891913
C	-3.412550	-3.924268	-0.107715
C	-3.459557	-1.497737	0.138401
C	3.722701	-9.759993	-0.730839
C	-3.547448	0.980108	0.263130
C	-4.155936	-2.763547	0.024297
C	-5.685731	-2.820595	0.078388
C	-5.651531	-0.287446	0.095161
C	-6.141951	-2.926440	1.550814
C	-6.266340	-4.008190	-0.712290
C	-6.224129	-1.529425	-0.565768
O	0.030335	-2.633502	-0.141111
O	2.059572	-3.549190	-0.399040
O	2.555147	-15.794036	-0.899756
O	4.536174	-14.662656	-0.980128
N	-0.077439	-13.359054	-0.633611
N	-4.192628	-0.329490	0.203658
S	1.173188	-10.277217	-0.594532
H	0.009631	-0.304955	-1.376683
H	-0.183893	1.355863	-0.782154
H	0.245600	0.759902	1.675252
H	-0.440656	-0.734680	2.339426
H	-0.328836	-7.854610	-0.414528
H	0.750221	-0.809048	1.025468
H	-1.498658	0.572083	-1.683736
H	-1.737895	-6.049554	-0.359540
H	-1.752701	1.884847	1.025800
H	2.108051	-5.941119	-0.513256
H	-2.436078	0.621100	2.057232
H	-3.406472	1.374845	-0.757954

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H      3.628336   -7.568477   -0.652491
H     -3.922470   -4.883493   -0.188907
H      4.338314  -12.339037   -0.868689
H     -4.231451    1.672133    0.775068
H      4.800402   -9.899212   -0.798329
H      4.832782  -15.597485   -1.042201
H     -5.752260   -2.104272    2.164611
H     -5.780721   -3.862464    1.995429
H     -5.912033   -4.009056   -1.751630
H     -6.017847   -4.978709   -0.265224
H     -5.917057    0.604381   -0.490583
H     -5.969473   -1.529478   -1.635487
H     -6.089178   -0.145211    1.097634
H     -7.239441   -2.915817    1.619857
H     -7.362490   -3.936936   -0.728004
H     -7.320899   -1.502780   -0.492840
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ADSORBED NKX-2593

Ti	24.894918	-10.901165	3.695983
Ti	22.148369	-10.420974	2.972005
Ti	23.645943	-7.836113	2.673995
Ti	22.829386	-10.633209	5.686707
Ti	24.422524	-4.636921	2.434482
Ti	26.572985	-8.943694	3.357878
Ti	26.896530	-6.121060	3.470941
Ti	24.397715	-8.066712	5.595108
Ti	25.422404	-4.926428	5.846383
O	23.478361	-11.536781	2.532803
O	26.640222	-10.861433	3.200919
O	22.167479	-8.839159	2.058613
O	23.333928	-9.212286	6.689730
O	21.355361	-10.962980	4.577009
O	24.173548	-11.749629	5.269383
O	26.222341	-5.036772	2.179986
O	25.015938	-9.165482	2.282345
O	27.866332	-7.679723	3.068984
O	25.434986	-7.284932	3.818879
O	27.120090	-5.273668	5.016861
O	23.681504	-6.258343	1.822581
O	23.008151	-7.123436	4.453984
O	24.293979	-4.668796	4.239074
O	25.730351	-9.406905	5.018492
O	25.397948	-3.721894	6.946127
O	24.907274	-6.681873	6.529239
O	23.396903	-9.574107	4.163955
O	16.918038	8.001654	1.051030
O	16.671275	6.106865	2.219307
O	22.778567	-3.374594	2.109843
O	24.795523	-2.885341	1.379344
C	14.505665	9.195306	0.189281
C	15.561377	10.779186	1.843489
C	18.640676	6.279981	0.824843
C	19.320336	7.159023	-0.020291
C	15.502269	10.367932	0.356221
C	17.555801	8.840725	0.160584
C	17.377228	6.724686	1.422848
C	19.032934	4.942666	1.192895
C	18.817833	8.440998	-0.357922
C	16.917077	10.045755	-0.158249
C	14.930009	11.517397	-0.497596
C	20.122553	4.201116	0.795090
C	19.481189	9.362535	-1.210415
C	17.667223	10.980272	-0.955802
C	15.887828	12.683103	-0.637676
C	18.954210	10.608793	-1.512989
C	19.689397	11.573423	-2.448388

C	17.908510	13.289321	-1.897810
C	21.871864	-0.739116	1.686322
C	19.175723	11.374599	-3.892667
C	21.215007	11.373767	-2.435415
C	19.398930	13.005564	-1.959658
C	23.107108	-1.160174	1.196042
C	23.971660	-0.321837	0.438296
C	23.563717	-2.498119	1.550038
C	20.323416	2.849102	1.239559
C	19.508182	2.067804	2.088494
C	19.991129	0.775118	2.279323
C	21.201531	0.501013	1.603330
N	17.169318	12.245540	-1.186894
N	24.649034	0.400012	-0.208083
S	21.719909	1.931481	0.705177
H	14.551501	8.778754	-0.825159
H	14.555638	11.034721	2.206130
H	15.942712	9.954130	2.455550
H	13.486343	9.573835	0.348448
H	18.325514	4.475700	1.880010
H	14.677921	8.385900	0.901139
H	16.214892	11.646205	2.005576
H	20.275406	6.853984	-0.455455
H	13.989920	11.866459	-0.048822
H	14.685877	11.135601	-1.499634
H	16.049814	13.188066	0.330466
H	20.864334	4.618601	0.110510
H	20.445388	9.069096	-1.624578
H	15.473092	13.436477	-1.322902
H	21.346312	-1.498254	2.271660
H	18.085667	11.477311	-3.965203
H	21.621286	11.428082	-1.417160
H	19.431516	10.369428	-4.250815
H	21.515186	10.414370	-2.874833
H	19.843014	13.142137	-0.963154
H	17.728159	14.239827	-1.373778
H	17.487867	13.407934	-2.911146
H	19.636349	12.105998	-4.572367
H	21.692793	12.161583	-3.033615
H	19.874623	13.736768	-2.627933
H	23.229782	-6.142772	4.464757
H	18.593896	2.443189	2.541510
H	19.505075	0.023234	2.898546