

**Supporting Information**

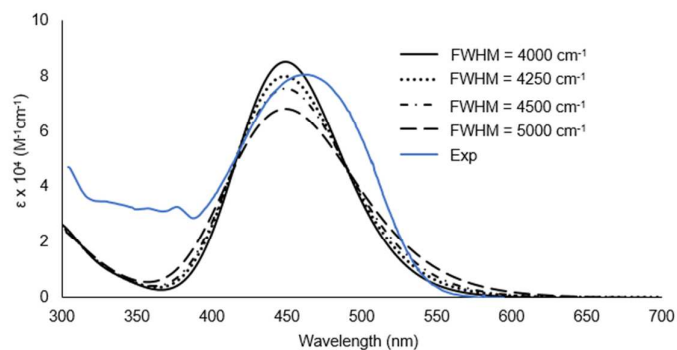
**The Effect of Donor Group Rigidification on the Electronic and Optical  
Properties of Arylamine-Based Metal-Free Dyes for Dye-Sensitized Solar  
Cells: A Computational Study**

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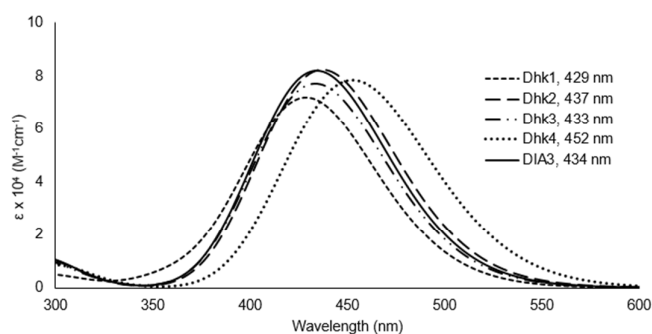
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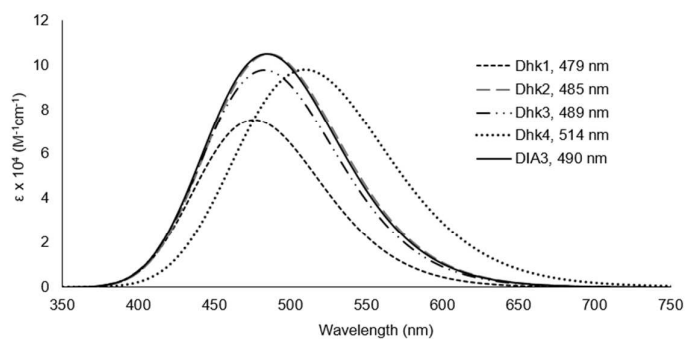
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**Figure S1.** Optimization of the half-bandwidth ( $\Delta_{1/2}$ ) for the absorption spectra of the reference dye calculated at TD-LC- $\omega$ PBE/6-31+G(d)//mPWHandHPW91/6-31G(d) in THF,  $\omega=0.175$  Bohr $^{-1}$ .



**Figure S2.** Simulated UV-Vis absorption spectra of the dyes calculated at TD-CAM-B3LYP/3-21+G(d)//SCC-DFTB+.



**Figure S3.** Simulated UV-Vis absorption spectra of the dye- $(\text{TiO}_2)_{38}$  complexes calculated at TD-CAM-B3LYP/3-21+G(d)//SCC-DFTB+.

**Table S1.** The calculated absorption wavelength ( $\lambda_{\text{abs}}$ ), oscillator strength ( $f$ ), and MO character of the major electronic transition with the corresponding percentage coefficient of dyes calculated at TD-CAM-B3LYP/3-21+G(d)//SCC-DFTB+.

Dye	$\lambda_{\text{abs}}$ (nm)	$f$	MO Character <sup>a</sup> (%)	
Dhk1	429	1.3963	H-1 $\rightarrow$ L+0 (46)	H-0 $\rightarrow$ L+0 (45)
Dhk2	437	1.6123	H-0 $\rightarrow$ L+0 (77)	H-1 $\rightarrow$ L+0 (16)
Dhk3	433	1.5085	H-0 $\rightarrow$ L+0 (79)	H-1 $\rightarrow$ L+0 (13)
Dhk4	452	1.5301	H-0 $\rightarrow$ L+0 (79)	H-1 $\rightarrow$ L+0 (14)
DIA3	433	1.6065	H-0 $\rightarrow$ L+0 (78)	H-1 $\rightarrow$ L+0 (15)

<sup>a</sup>H = HOMO and L = LUMO.

**Table S2.** Cartesian Coordinates of the Dhk1 dye optimized at SSC-DFTB+.

C	-5.21867	3.49984	1.12004	C	3.37897	0.96750	-0.91621
C	-4.51783	2.35780	0.74091	H	1.55288	1.87460	-1.76911
C	-5.20541	1.19204	0.33908	C	3.71750	-0.00617	0.01028
C	-6.61877	1.16864	0.37375	H	4.12725	1.54449	-1.47067
C	-7.29737	2.33317	0.75826	C	-8.27422	-0.46925	1.27341
C	-6.61480	3.49685	1.11731	H	-8.97107	0.35530	1.51526
C	-7.42335	-0.07641	0.04267	H	-8.90538	-1.34098	1.01693
C	-6.53026	-1.24417	-0.33961	C	-8.38082	0.23343	-1.13199
C	-5.12104	-1.13943	-0.38948	H	-9.00779	-0.65480	-1.33691
C	-4.35633	-2.23947	-0.83489	H	-9.07680	1.03956	-0.83212
H	-3.26673	-2.14740	-0.92563	C	-7.42753	-0.79140	2.47861
C	-4.97243	-3.44100	-1.17528	H	-8.05566	-1.07312	3.33343
C	-6.36028	-3.56458	-1.08871	H	-6.74690	-1.62670	2.26756
C	-7.12234	-2.46658	-0.68540	H	-6.81917	0.07340	2.77426
H	-4.66729	4.39882	1.42567	C	-7.64456	0.63676	-2.38450
H	-3.42085	2.36392	0.76640	H	-6.97322	-0.16410	-2.72086
H	-8.39608	2.33254	0.78310	H	-8.34856	0.85393	-3.19812
H	-7.17325	4.39450	1.41182	H	-7.03794	1.53543	-2.21122
H	-4.36110	-4.28687	-1.51645	C	5.03393	-0.41694	0.39670
H	-6.85176	-4.50997	-1.35185	S	6.48900	0.32456	-0.31021
H	-8.21596	-2.56621	-0.64347	C	5.36805	-1.39537	1.32785
N	-4.47988	0.05733	-0.04520	C	7.52993	-0.72653	0.69206
C	-3.05496	0.12438	-0.09665	C	6.75901	-1.56652	1.49131
C	-2.27555	-0.71188	0.72322	H	4.61644	-1.97236	1.87774
C	-2.41922	1.02529	-0.97065	C	8.95633	-0.70783	0.68036
C	-0.88706	-0.64938	0.66310	H	7.20262	-2.29229	2.18260
H	-2.76575	-1.41066	1.41322	C	9.77977	0.08880	-0.07900
C	-1.03061	1.08603	-1.02343	H	9.46071	-1.41361	1.36055
H	-3.02308	1.67610	-1.61603	C	9.29308	1.06037	-1.01665
C	-0.23613	0.24834	-0.21011	C	11.24403	-0.05672	0.07353
H	-0.28965	-1.30476	1.31112	N	8.95140	1.85115	-1.78047
H	-0.55102	1.79002	-1.71605	O	11.78367	-0.84601	0.83437
C	1.21409	0.31221	-0.27733	O	11.99861	0.77826	-0.71845
C	1.98160	1.14368	-1.07501	H	12.94604	0.59675	-0.53453
S	2.25223	-0.74431	0.72336				

**Table S3.** Cartesian Coordinates of the **Dhk2** dye optimized at SSC-DFTB+.

C	8.39157	3.20363	0.03462	H	-1.07591	2.97295	-0.08995
C	7.13695	3.82498	0.13213	C	-3.13334	0.30002	0.03981
C	5.94893	3.09335	0.13037	H	-3.63060	2.42342	-0.05544
C	6.02715	1.69270	0.01856	C	3.02358	-2.68967	-1.17188
C	7.30683	1.06113	-0.05406	H	1.92995	-2.82905	-1.07986
C	8.48773	1.81667	-0.05103	H	3.46733	-3.70243	-1.13380
H	9.30095	3.81852	0.03892	C	3.15083	-2.60806	1.33115
H	7.08528	4.91857	0.21787	H	2.05286	-2.74341	1.35746
H	5.00351	3.63415	0.23394	H	3.58954	-3.62366	1.31291
H	9.46597	1.32183	-0.11061	C	3.60499	-1.87858	2.57003
C	5.67950	-0.53759	-0.05256	H	4.69667	-1.76507	2.58157
C	5.05440	-1.78874	-0.04944	H	3.16035	-0.87598	2.62132
C	5.90042	-2.90319	-0.10366	H	3.31074	-2.42695	3.47378
C	7.29852	-2.75606	-0.15910	C	3.34659	-2.04140	-2.49432
C	7.90807	-1.50107	-0.15494	H	4.43070	-1.92392	-2.61961
C	7.08178	-0.36679	-0.09817	H	2.97184	-2.64944	-3.32736
H	5.47124	-3.91479	-0.10030	H	2.88818	-1.04640	-2.56674
H	7.92333	-3.65837	-0.20125	C	-4.42469	-0.31672	0.06635
H	9.00112	-1.40658	-0.19179	S	-5.92111	0.64471	0.00245
C	3.64175	0.74001	-0.01450	C	-4.70301	-1.67878	0.13616
C	3.54570	-1.87201	0.03092	C	-6.90148	-0.84854	0.07159
C	2.90824	-0.48099	0.01903	C	-6.08253	-1.97286	0.13973
C	2.93779	1.96046	-0.08333	H	-3.91935	-2.44277	0.18288
C	1.51256	-0.41715	0.03200	C	-8.32659	-0.88817	0.05256
C	1.54939	1.99329	-0.07939	H	-6.48409	-2.99144	0.18969
H	3.47516	2.90791	-0.15970	C	-9.19589	0.17465	-0.02309
C	0.80242	0.80070	-0.00779	H	-8.78858	-1.88790	0.10034
H	0.93792	-1.35326	0.07144	C	-8.76546	1.54200	-0.09301
H	1.03881	2.96317	-0.13442	C	-10.64933	-0.09688	-0.03796
N	5.03974	0.69663	-0.00033	N	-8.47038	2.65339	-0.15113
C	-0.64876	0.83064	0.00475	O	-11.14509	-1.21278	0.01417
C	-1.46379	1.94961	-0.04131	O	-11.45048	1.01983	-0.11860
S	-1.62541	-0.66495	0.07904	H	-12.38619	0.72168	-0.12370
C	-2.84972	1.65545	-0.02284				

**Table S4.** Cartesian Coordinates of the **Dhk3** dye optimized at SSC-DFTB+.

C	-1.58298	1.35519	-0.03833	H	-2.84499	-3.44536	-1.01825
C	-2.97716	1.48499	-0.04639	H	-4.52343	-4.00575	-1.02512
C	-3.78554	0.32435	-0.01913	C	-4.10827	-2.43659	-2.43670
C	-3.25886	-0.97259	0.02753	H	-3.46570	-1.55296	-2.54486
C	-1.86754	-1.08191	0.03545	H	-3.87539	-3.12861	-3.25583
C	-1.02264	0.06219	-0.00094	H	-5.15088	-2.11245	-2.55121
C	-4.19972	-2.15657	0.08511	C	-4.24060	-2.09310	2.62344
C	-5.66145	-1.71157	0.01887	H	-4.05102	-2.66681	3.53943
C	-6.09252	-0.35787	-0.05200	H	-3.60502	-1.19822	2.64532
C	-7.46808	-0.07431	-0.15747	H	-5.28803	-1.76456	2.63885
H	-7.82033	0.95460	-0.25202	C	0.42114	-0.11450	0.00552
C	-8.41183	-1.09981	-0.16043	C	1.12519	-1.30675	-0.01988
C	-8.00043	-2.42803	-0.06060	S	1.53898	1.28049	0.04719
C	-6.63780	-2.71756	0.02046	C	2.53341	-1.14751	-0.00829
H	-0.93656	2.24239	-0.06139	H	0.64357	-2.29009	-0.05121
H	-1.40896	-2.07916	0.07703	C	2.94703	0.17481	0.02809
H	-9.47836	-0.85315	-0.24141	H	3.23581	-1.98834	-0.02559
H	-8.73734	-3.24104	-0.05630	C	4.29186	0.66424	0.04664
H	-6.32514	-3.76881	0.08600	S	5.68811	-0.43841	-0.00078
N	-5.12987	0.66487	-0.03166	C	4.70087	1.99383	0.09929
H	-6.93279	5.00264	-0.00333	C	6.80877	0.95387	0.05100
C	-6.07816	4.31334	-0.02666	C	6.10238	2.15309	0.10253
C	-4.77648	4.83707	-0.06474	H	3.99469	2.83043	0.13539
C	-6.32172	2.93979	-0.01243	C	8.23065	0.85380	0.03524
C	-3.67419	3.98616	-0.07747	H	6.60069	3.12856	0.14055
H	-4.63080	5.92495	-0.07483	C	8.99163	-0.29036	-0.02438
C	-5.21971	2.06482	-0.04462	H	8.78891	1.80376	0.07164
H	-7.35875	2.59535	0.03676	C	8.42984	-1.60997	-0.07743
C	-3.89565	2.60194	-0.06398	C	10.46442	-0.16348	-0.03818
H	-2.65193	4.38661	-0.09374	N	8.02921	-2.68862	-0.12083
C	-3.95496	-2.92861	1.40133	O	11.06832	0.89818	0.00604
H	-4.58271	-3.83955	1.41511	O	11.15173	-1.35473	-0.10828
H	-2.90400	-3.27452	1.42162	H	12.11214	-1.14997	-0.11381
C	-3.89305	-3.09986	-1.09979				

**Table S5.** Cartesian Coordinates of the **Dhk4** dye optimized at SSC-DFTB+.

C	-7.95668	-1.78200	-0.04235	H	-2.05616	-2.93873	-1.19151
C	-7.21319	-0.60432	-0.03471	H	-3.59144	-3.81806	-1.20365
C	-5.80344	-0.65306	-0.01763	C	-3.59317	-2.08688	2.54544
C	-5.13506	-1.89852	-0.01011	H	-3.27501	-2.66066	3.42523
C	-5.91052	-3.06555	-0.01788	H	-3.13987	-1.08879	2.60877
C	-7.30649	-3.01801	-0.03372	H	-4.68333	-1.96608	2.59392
C	-3.61868	-2.00905	0.00821	C	-3.53221	-2.12436	-2.52674
C	-2.94799	-0.64360	0.00845	H	-3.08181	-1.12523	-2.59302
C	-3.69220	0.56192	0.00161	H	-3.18882	-2.70929	-3.38949
C	-3.01679	1.80379	0.01081	H	-4.62129	-2.00993	-2.60538
H	-3.59987	2.73380	0.00838	H	-7.72232	5.16689	-0.02735
C	-1.63045	1.85652	0.02282	C	0.58314	0.72173	0.03293
C	-0.86632	0.66928	0.02609	C	1.38229	1.85414	0.04082
C	-1.55464	-0.56410	0.02022	S	1.58291	-0.76085	0.02532
H	-9.05350	-1.73388	-0.05540	C	2.77198	1.58066	0.03989
H	-7.72042	0.36912	-0.04190	H	0.97989	2.87295	0.04644
H	-5.41176	-4.04484	-0.01098	C	3.07753	0.22807	0.03123
H	-7.88704	-3.94940	-0.03941	H	3.54112	2.36121	0.04497
H	-1.13051	2.83373	0.02942	C	4.37705	-0.36894	0.02398
H	-0.96635	-1.49270	0.02538	S	5.85874	0.61727	0.02040
N	-5.08061	0.54155	-0.01068	C	4.67659	-1.72900	0.01559
C	-5.79705	1.79003	-0.01546	C	6.86255	-0.86318	0.00534
C	-6.18284	2.37639	1.19904	C	6.05982	-2.00190	0.00528
C	-6.10202	2.41386	-1.23424	H	3.90401	-2.50554	0.01601
C	-6.87410	3.58904	1.18792	C	8.28717	-0.87853	-0.01048
H	-5.93967	1.88111	2.14772	H	6.47670	-3.01564	-0.00296
C	-6.79395	3.62618	-1.23153	C	9.13921	0.20193	-0.01436
H	-5.79626	1.94796	-2.17968	H	8.76640	-1.87125	-0.02424
C	-7.17912	4.21308	-0.02395	C	8.68671	1.56370	0.00381
H	-7.17728	4.05294	2.13574	C	10.59630	-0.04258	-0.04099
H	-7.03507	4.11871	-2.18268	N	8.37587	2.67241	0.01869
C	-3.18440	-2.78539	1.27326	O	11.11347	-1.15022	-0.05869
H	-3.62369	-3.80034	1.24660	O	11.37823	1.09174	-0.04679
H	-2.08666	-2.92287	1.25833	H	12.31887	0.81061	-0.06669
C	-3.15328	-2.80277	-1.23464				

**Table S6.** Cartesian Coordinates of the **DIA3** dye optimized at SSC-DFTB+.

C	-0.34257	0.77162	-0.07464	H	-9.10626	-0.72283	-0.93964
C	-1.06668	1.99017	-0.01563	H	-8.30631	-2.30084	-0.95230
C	-2.45650	2.03467	0.00442	C	-7.09523	-0.71648	2.66475
C	-3.17380	0.82241	-0.04430	H	-6.12128	-1.22300	2.66806
C	-2.45334	-0.41322	-0.07915	H	-6.91325	0.36624	2.67355
C	-1.05622	-0.44112	-0.09878	H	-7.61859	-0.98016	3.59255
H	-0.51503	2.93850	0.02267	C	-7.52425	-0.90192	-2.38647
H	-2.94188	3.01258	0.07668	H	-8.19317	-1.23057	-3.19192
H	-0.52388	-1.40119	-0.12561	H	-7.35699	0.17691	-2.50256
C	-4.69207	-0.84487	-0.01496	H	-6.55962	-1.40950	-2.51695
C	-5.90346	-1.54179	0.04705	C	1.11033	0.78549	-0.08587
C	-5.81377	-2.93902	0.05066	C	1.94297	1.89148	-0.05103
C	-4.56815	-3.59130	-0.00489	S	2.06374	-0.72618	-0.13585
C	-3.36763	-2.88279	-0.05709	C	3.32428	1.57483	-0.05685
C	-3.43010	-1.47975	-0.05987	H	1.57329	2.92208	-0.01818
H	-6.72933	-3.54473	0.10128	C	3.58664	0.21440	-0.09856
H	-4.54607	-4.68939	0.00027	H	4.11705	2.33066	-0.02926
H	-2.40445	-3.40831	-0.09083	C	4.86842	-0.42238	-0.10189
C	-5.68845	1.34873	-0.04188	S	6.37687	0.51805	-0.01670
C	-7.20438	-0.77385	0.12830	C	5.12828	-1.78881	-0.15860
C	-6.96824	0.73525	0.05091	C	7.33701	-0.98941	-0.05872
C	-5.59845	2.74845	-0.17011	C	6.50336	-2.10248	-0.13537
C	-8.09900	1.56394	0.06128	H	4.33436	-2.54155	-0.21547
C	-6.74412	3.54180	-0.16503	C	8.76081	-1.04683	-0.01588
H	-4.62933	3.23654	-0.29211	H	6.89104	-3.12707	-0.17249
C	-8.00101	2.95264	-0.03532	C	9.64080	0.00692	0.06719
H	-9.09609	1.11004	0.14556	H	9.21176	-2.05210	-0.05034
H	-6.64852	4.63072	-0.26414	C	9.22531	1.37946	0.12398
H	-8.90745	3.57104	-0.02308	C	11.09097	-0.27816	0.10317
N	-4.54213	0.53791	-0.02392	N	8.94466	2.49504	0.17319
C	-7.90852	-1.11778	1.46027	O	11.57830	-1.39810	0.05935
H	-8.89620	-0.62002	1.49245	O	11.90045	0.83235	0.19334
H	-8.10669	-2.20605	1.48823	H	12.83354	0.52693	0.21121
C	-8.11959	-1.21353	-1.03667				

**Table S7.** Cartesian Coordinates of the  $\text{Dhk1}-(\text{TiO}_2)_{38}$  clusters optimized at SSC-DFTB+.

C	19.40898	-2.47293	1.28143	S	7.45153	-0.30899	-0.34545
C	18.60823	-1.75668	0.39544	C	8.70974	1.98043	-0.06970
C	19.18000	-1.07401	-0.69994	C	6.50228	1.17278	-0.02964
C	20.58396	-1.07615	-0.86817	C	7.34073	2.27894	0.08841
C	21.36472	-1.80437	0.03985	H	9.50569	2.73044	-0.00961
C	20.79278	-2.50957	1.10028	H	6.95998	3.28842	0.28195
C	21.27544	-0.30040	-1.97590	C	5.08156	1.22469	0.08006
C	20.28204	0.43406	-2.85956	C	4.18783	0.18750	-0.05141
C	18.88529	0.37120	-2.64959	H	4.64636	2.21620	0.28917
C	18.01473	1.01664	-3.55440	C	2.72765	0.43829	0.09677
H	16.92859	0.93008	-3.42503	C	4.59596	-1.16106	-0.32881
C	18.52031	1.75408	-4.62199	O	1.93897	-0.56208	-0.12422
C	19.89976	1.85131	-4.81373	O	2.37608	1.63518	0.38565
C	20.76206	1.18443	-3.94169	N	4.86573	-2.25868	-0.54809
H	18.94596	-3.00284	2.12423	Ti	0.04088	-1.06833	0.66897
H	17.52393	-1.71728	0.55890	O	-1.88957	-1.10716	0.64469
H	22.45693	-1.82018	-0.08122	O	-0.21627	-1.37414	-1.28295
H	21.42945	-3.07382	1.79346	O	0.07584	-2.94990	1.17045
H	17.82811	2.25230	-5.31356	O	-0.01856	0.73149	1.29510
H	20.30508	2.43247	-5.65164	Ti	-2.22514	-0.84100	-1.36135
H	21.84562	1.24795	-4.11400	Ti	-3.69817	-0.96466	1.68249
N	18.35490	-0.36350	-1.58115	H	0.37272	-0.88078	-1.88739
C	16.94062	-0.39739	-1.39329	Ti	-0.51885	-4.74930	0.82380
C	16.23240	0.78832	-1.12529	Ti	0.70287	-2.71364	3.12684
C	16.24380	-1.61685	-1.47786	Ti	0.40073	2.43989	0.55069
C	14.85275	0.75170	-0.95121	O	-2.85313	-2.81311	-1.47565
H	16.77187	1.74115	-1.04975	O	-1.75621	0.95393	-1.68488
C	14.86469	-1.64769	-1.29999	O	-2.15461	-1.08005	-3.30241
H	16.79092	-2.54360	-1.69323	O	-4.05833	-0.43990	-0.80586
C	14.14093	-0.46414	-1.03619	O	-5.57961	-0.55769	1.48083
H	14.31133	1.68338	-0.73840	O	-3.62310	-0.84983	3.56568
H	14.33547	-2.60627	-1.37808	O	-3.96963	-2.75491	1.48381
C	12.69839	-0.50217	-0.86691	O	-3.07455	0.94950	1.86610
C	11.87443	-1.61346	-0.93045	Ti	0.24945	-5.95819	2.88277
S	11.74798	0.97753	-0.55139	Ti	-2.44568	-4.58789	-1.13456
C	10.50047	-1.32415	-0.74049	O	-2.33447	-4.69546	0.84187
H	12.24587	-2.62745	-1.11414	O	-0.53558	-4.75401	-0.98582
C	10.23718	0.01965	-0.52352	O	-0.05477	-6.59658	1.24117
H	9.71410	-2.08673	-0.76261	O	1.31200	-1.03959	2.49195
C	22.24800	0.72438	-1.34627	O	1.42409	-2.81939	4.86952
H	23.01301	0.18756	-0.75417	Ti	-0.26933	-2.67382	5.48232
H	22.79421	1.25019	-2.15211	O	-0.97752	-2.42475	3.81594
C	22.09766	-1.28132	-2.84435	O	1.31346	-4.55724	2.64790
H	22.64946	-0.71308	-3.61669	Ti	-1.38226	2.69242	-1.46432
H	22.86454	-1.77021	-2.21439	O	-1.49025	2.68741	0.52597
C	21.53909	1.72858	-0.47319	O	0.48029	2.59792	-1.25457
H	22.25024	2.45098	-0.05240	O	0.46953	4.26334	1.16548
H	20.78787	2.28650	-1.04784	Ti	-3.24162	-2.47401	-3.52900
H	21.02598	1.23160	0.36050	Ti	-5.74689	-0.53965	-0.29154
C	21.23506	-2.32903	-3.50138	Ti	-2.92607	0.80820	3.94989
H	20.49140	-1.86659	-4.16346	Ti	-4.41718	-4.52666	1.56676
H	21.84481	-3.01630	-4.10180	Ti	-3.39260	2.62275	1.24358
H	20.69624	-2.92121	-2.74989	O	0.23769	-6.83931	4.53215
C	8.96110	0.63261	-0.31115	Ti	-1.17418	-5.76968	5.03275



O	-1.38943	-5.02973	3.24739
Ti	-3.34240	-5.40864	-3.58088
O	-2.92969	-6.25086	-2.06066
Ti	0.81657	0.74277	3.23720
O	-0.87852	-4.33658	6.11289
O	-0.53116	-1.17697	6.47693
O	-1.27622	3.43474	-3.29333
Ti	0.15227	6.08287	1.28711
Ti	0.87907	4.21997	3.22353
O	-2.11197	-4.13432	-3.65001
O	-3.62007	-2.34140	-5.32514
O	-5.03000	-1.69610	-3.22011
O	-6.25514	-2.35461	-0.74952
O	-6.49245	1.26885	-0.48437
O	-3.63126	2.67754	3.81316
O	-2.59617	0.65024	5.74468
O	-1.02267	0.79452	3.71961
Ti	-3.25764	-5.72881	3.42380
Ti	-6.19568	-4.25626	-0.44765
O	-6.32967	-4.47964	1.32514
O	-4.29221	-4.34173	3.57193
O	-4.44672	-4.69995	-0.50344
O	-3.93338	-6.46613	1.98435
Ti	-5.42917	2.88330	-0.27040
O	-5.29568	2.92101	1.50281
O	-3.77440	2.31321	-0.62806
O	-2.96628	4.45462	1.81801
O	-2.78774	-6.58025	5.07125
O	-3.98718	-6.09776	-5.19616
Ti	-5.51362	-5.05564	-5.09112
O	-4.98491	-4.36572	-3.31225
O	1.54620	2.47517	2.85115
O	1.19550	0.45121	4.95309
Ti	-0.68697	0.50469	5.64895
Ti	-2.30443	4.86868	-3.13229
O	-1.50696	6.73694	1.61438
O	1.23960	6.06329	2.79097
O	0.28626	6.65660	-0.44626
O	1.03669	4.45139	5.08785

Ti	-0.55603	3.61875	5.42407
O	-0.93025	3.57405	3.51682
Ti	-5.44948	-1.86714	-5.16954
Ti	-6.85779	-1.91723	-2.79353
Ti	-6.71116	1.49224	-2.51684
Ti	-2.73417	4.25713	3.89591
Ti	-6.76660	-5.04840	-2.80855
O	-6.77593	-5.94199	-1.27400
O	-4.79863	4.77614	-0.48342
Ti	-3.30663	6.24093	2.00923
O	-5.78817	-3.63071	-6.08837
O	-7.03153	-5.88641	-4.44237
O	-0.36887	2.16211	6.47742
Ti	-1.53351	6.35222	-0.94529
O	-2.09770	4.62515	-1.07188
O	-2.97998	5.28487	-4.90254
O	-1.53885	6.57440	-2.73958
Ti	-4.53153	4.42491	-4.63999
O	-4.10811	4.04003	-2.85638
O	-2.11740	4.49011	5.69360
O	-5.50226	-0.13470	-5.83168
O	-7.27941	-1.95818	-4.54868
O	-7.77042	-3.62942	-2.38815
O	-7.43845	-0.27766	-2.21360
Ti	-5.67323	1.40823	-4.85672
O	-5.02941	1.20387	-3.14557
O	-7.35417	1.78097	-4.26333
O	-6.75072	3.44917	-1.85440
O	-3.38733	6.07271	3.80354
Ti	-5.76225	5.00093	-2.32658
Ti	-4.83830	6.56019	-0.24101
O	-5.06582	6.79723	1.55669
O	-3.13692	7.21157	-0.38240
O	-4.86191	2.89290	-5.59569
O	-6.01872	5.36957	-4.14685
O	-6.04390	6.74533	-1.63956

**Table S8.** Cartesian Coordinates of the  $\text{Dhk2-(TiO}_2\text{)}_{38}$  clusters optimized at SSC-DFTB+.

C	21.62314	-3.73158	-2.49552	C	6.62425	0.90903	-0.48484
C	20.33939	-4.29827	-2.48734	C	7.50764	1.98088	-0.37103
C	19.19414	-3.52975	-2.27566	H	9.68753	2.34647	-0.48122
C	19.34648	-2.14758	-2.05967	H	7.16889	3.00367	-0.16900
C	20.65377	-1.57164	-2.08514	C	5.20988	1.01384	-0.34783
C	21.79081	-2.36282	-2.29978	C	4.27388	0.01135	-0.46359
H	22.49692	-4.37386	-2.66588	H	4.81665	2.01869	-0.12041
H	20.22840	-5.37778	-2.65565	C	2.83156	0.31353	-0.26186
H	18.22169	-4.03033	-2.29702	C	4.62267	-1.34926	-0.76188
H	22.79021	-1.90862	-2.31585	O	1.99753	-0.65949	-0.44219
C	19.11568	0.07584	-1.73361	O	2.53124	1.52396	0.02960
C	18.55754	1.34244	-1.53349	N	4.84333	-2.45405	-0.99927
C	19.45719	2.41391	-1.47392	Ti	0.15656	-1.11754	0.49319
C	20.84277	2.21166	-1.60845	O	-1.77155	-1.10614	0.61370
C	21.38520	0.94239	-1.81167	O	-0.25596	-1.43055	-1.43113
C	20.50347	-0.14850	-1.87735	O	0.17836	-2.99594	1.00741
H	19.08053	3.43497	-1.32174	O	0.18837	0.68522	1.11421
H	21.51133	3.08132	-1.55503	Ti	-2.25000	-0.84405	-1.36312
H	22.46873	0.80370	-1.91934	Ti	-3.49171	-0.91262	1.78397
C	17.02514	-1.11250	-1.67821	H	0.29943	-0.95690	-2.08149
C	17.05719	1.48865	-1.40827	Ti	-0.48420	-4.78170	0.71839
C	16.35566	0.13124	-1.48696	Ti	0.95976	-2.76624	2.90804
C	16.26586	-2.30172	-1.69615	Ti	0.59507	2.37773	0.32658
C	14.96484	0.12467	-1.35759	O	-2.93631	-2.80007	-1.41332
C	14.88368	-2.27816	-1.56378	O	-1.76101	0.93603	-1.73520
H	16.75452	-3.27180	-1.80469	O	-2.33582	-1.09682	-3.30196
C	14.19780	-1.05813	-1.40099	O	-4.02560	-0.39272	-0.67409
H	14.43956	1.08015	-1.21935	O	-5.37157	-0.45669	1.72169
H	14.32978	-3.22544	-1.58367	O	-3.27335	-0.79215	3.65599
N	18.41501	-1.12287	-1.83016	O	-3.82352	-2.69600	1.61900
C	12.75237	-1.02585	-1.27588	O	-2.80704	0.98489	1.90946
C	11.87966	-2.09877	-1.36167	Ti	0.40817	-5.99903	2.72219
S	11.86272	0.49607	-0.98319	Ti	-2.54974	-4.58272	-1.08980
C	10.51675	-1.74785	-1.20264	O	-2.29168	-4.68271	0.87325
H	12.20965	-3.12777	-1.54051	O	-0.63831	-4.79610	-1.08451
C	10.30841	-0.39368	-0.98764	O	-0.03675	-6.63819	1.11345
H	9.69739	-2.47431	-1.24327	O	1.56281	-1.11255	2.21776
C	16.73020	2.16148	-0.05623	O	1.80791	-2.88296	4.59220
H	15.64210	2.35014	0.01064	Ti	0.17029	-2.69042	5.33034
H	17.21828	3.15379	-0.02566	O	-0.65564	-2.43031	3.72102
C	16.54433	2.40044	-2.54575	O	1.48602	-4.62713	2.39650
H	15.46052	2.58054	-2.41333	Ti	-1.32714	2.66510	-1.55217
H	17.03601	3.38781	-2.45963	O	-1.28686	2.67260	0.43986
C	16.80190	1.81998	-3.91327	O	0.54288	2.52360	-1.48044
H	17.87583	1.66429	-4.07831	O	0.75184	4.20222	0.92247
H	16.29805	0.85148	-4.03087	Ti	-3.47297	-2.46271	-3.43316
H	16.43124	2.49253	-4.69711	Ti	-5.67225	-0.44511	-0.03305
C	17.17945	1.33638	1.12307	Ti	-2.50763	0.84852	3.97719
H	18.26357	1.16699	1.09358	Ti	-4.30852	-4.45465	1.75133
H	16.93998	1.84352	2.06621	Ti	-3.12974	2.66171	1.29942
H	16.68434	0.35642	1.12925	O	0.49800	-6.87161	4.37384
C	9.05872	0.27193	-0.78418	Ti	-0.84448	-5.76342	4.97188
S	7.51203	-0.60832	-0.81439	O	-1.17439	-5.02650	3.20301
C	8.86196	1.62892	-0.53939	Ti	-3.65271	-5.39398	-3.45299

O	-3.14461	-6.23843	-1.96320
Ti	1.16835	0.68496	2.98662
O	-0.43035	-4.33414	6.01727
O	0.02229	-1.18317	6.33281
O	-1.33830	3.39661	-3.38878
Ti	0.49244	6.02992	1.05317
Ti	1.31511	4.15986	2.94369
O	-2.39903	-4.15293	-3.62696
O	-3.98366	-2.33160	-5.19663
O	-5.21226	-1.63619	-2.99635
O	-6.26018	-2.24887	-0.43586
O	-6.38469	1.38086	-0.18188
O	-3.17483	2.73471	3.87946
O	-2.04782	0.68997	5.74320
O	-0.62756	0.78522	3.60576
Ti	-3.04158	-5.67533	3.52310
Ti	-6.22736	-4.14932	-0.12436
O	-6.23209	-4.35847	1.65517
O	-4.02602	-4.26064	3.73893
O	-4.49985	-4.63961	-0.30930
O	-3.84461	-6.40407	2.14616
Ti	-5.26634	2.96747	-0.06016
O	-4.99988	3.01187	1.69772
O	-3.65876	2.35120	-0.53620
O	-2.61509	4.48452	1.82735
O	-2.47168	-6.53025	5.13664
O	-4.43675	-6.07548	-5.00886
Ti	-5.92302	-4.99244	-4.79632
O	-5.24265	-4.30655	-3.06817
O	1.90886	2.39729	2.53597
O	1.66802	0.39262	4.67134
Ti	-0.15495	0.49708	5.50605
Ti	-2.31684	4.85591	-3.16188
O	-1.12025	6.72896	1.49928
O	1.68918	5.99076	2.47107
O	0.51086	6.59035	-0.68961
O	1.61703	4.39818	4.78952

Ti	0.03444	3.60651	5.24950
O	-0.48246	3.56054	3.37639
Ti	-5.78256	-1.80765	-4.90665
Ti	-7.00768	-1.80740	-2.43069
Ti	-6.75134	1.59811	-2.19323
Ti	-2.23524	4.29126	3.88384
Ti	-6.99843	-4.93837	-2.42620
O	-6.91405	-5.82393	-0.88950
O	-4.60380	4.84129	-0.33520
Ti	-2.89691	6.27960	2.03087
O	-6.23596	-3.56773	-5.78230
O	-7.40877	-5.77866	-4.02841
O	0.26446	2.15090	6.29588
Ti	-1.34835	6.33071	-1.04839
O	-1.96288	4.61793	-1.12065
O	-3.11251	5.27875	-4.88016
O	-1.48315	6.54418	-2.83879
Ti	-4.66084	4.45964	-4.49605
O	-4.11445	4.07302	-2.74681
O	-1.48050	4.51805	5.62890
O	-5.83984	-0.07852	-5.57709
O	-7.56218	-1.84735	-4.14840
O	-7.93126	-3.49158	-1.94174
O	-7.49982	-0.14984	-1.82144
Ti	-5.89526	1.47387	-4.60382
O	-5.12989	1.26163	-2.94445
O	-7.51653	1.89416	-3.88862
O	-6.68941	3.55902	-1.54438
O	-2.84791	6.12259	3.82723
Ti	-5.69878	5.08041	-2.10117
Ti	-4.58352	6.62682	-0.10145
O	-4.67138	6.87636	1.70667
O	-2.88213	7.23512	-0.37283
O	-5.10298	2.93192	-5.41313
O	-6.08192	5.44550	-3.89980
O	-5.88538	6.83487	-1.40731

**Table S8.** Cartesian Coordinates of the  $\text{Dhk3-(TiO}_2\text{)}_{38}$  clusters optimized at SSC-DFTB+.

C	14.98535	0.94660	-0.77374	C	6.62077	1.36993	-0.17950
C	16.38196	0.94829	-0.86934	C	7.45911	2.46200	0.03719
C	17.04147	-0.15785	-1.45589	H	9.62168	2.92635	-0.03196
C	16.36170	-1.27192	-1.96482	H	7.07880	3.44509	0.33795
C	14.97033	-1.25754	-1.85651	C	5.20351	1.40257	-0.03768
C	14.27367	-0.16687	-1.26511	C	4.31709	0.35984	-0.18633
C	17.14840	-2.39215	-2.61074	H	4.76398	2.37783	0.23015
C	18.65398	-2.13392	-2.53393	C	2.86042	0.58396	0.01124
C	19.24715	-0.97477	-1.96205	C	4.73269	-0.97434	-0.51685
C	20.65036	-0.87499	-1.89664	O	2.09115	-0.45014	-0.10407
H	21.12747	-0.01559	-1.42157	O	2.48539	1.78749	0.23937
C	21.46352	-1.87898	-2.41894	N	5.00501	-2.06112	-0.78229
C	20.89126	-3.00254	-3.01373	Ti	0.22742	-0.93946	0.76734
C	19.50151	-3.12069	-3.05688	O	-1.70320	-1.03245	0.75938
H	14.45177	1.79267	-0.32074	O	-0.03452	-1.44976	-1.14204
H	14.39277	-2.10560	-2.24892	O	0.31186	-2.76400	1.44584
H	22.55471	-1.77745	-2.35797	O	0.11492	0.90655	1.23212
H	21.52446	-3.79407	-3.43384	Ti	-2.05117	-0.96470	-1.26000
H	19.06225	-4.01772	-3.51457	Ti	-3.51125	-0.84221	1.78889
N	18.41371	0.03807	-1.45898	H	0.54519	-1.01388	-1.79756
H	20.71794	3.83961	0.05788	Ti	-0.23442	-4.60320	1.27229
C	19.79074	3.27252	-0.09933	Ti	0.93974	-2.32830	3.36639
C	18.56818	3.83410	0.30067	Ti	0.49208	2.54969	0.33315
C	19.86558	2.01449	-0.69733	O	-2.62948	-2.95549	-1.18631
C	17.37515	3.14594	0.09463	O	-1.62658	0.80352	-1.74871
H	18.55655	4.82685	0.76891	O	-1.98242	-1.38121	-3.17113
C	18.67167	1.29501	-0.89189	O	-3.89305	-0.56143	-0.73547
H	20.84667	1.64147	-1.00550	O	-5.40358	-0.50491	1.56001
C	17.42668	1.87964	-0.50490	O	-3.43654	-0.55244	3.65344
H	16.41255	3.58353	0.39032	O	-3.73652	-2.64981	1.75924
C	16.72131	-2.51661	-4.09071	O	-2.93916	1.09608	1.79315
H	17.23654	-3.38146	-4.54946	Ti	0.57314	-5.59235	3.43103
H	15.63858	-2.74156	-4.13186	Ti	-2.17117	-4.67815	-0.68193
C	16.81601	-3.71925	-1.89248	O	-2.05086	-4.59756	1.29549
H	15.72982	-3.91069	-1.98121	O	-0.25652	-4.77863	-0.52835
H	17.31991	-4.55661	-2.41043	O	0.28170	-6.39034	1.85877
C	17.21432	-3.70445	-0.43836	O	1.50636	-0.70854	2.57035
H	16.69664	-2.90205	0.10323	O	1.66748	-2.25304	5.10819
H	16.96183	-4.65734	0.04362	Ti	-0.02779	-2.09774	5.71387
H	18.29476	-3.54381	-0.32866	O	-0.74603	-2.02084	4.03495
C	17.01406	-1.26862	-4.88452	O	1.59853	-4.19188	3.05926
H	16.69885	-1.38924	-5.92860	Ti	-1.30072	2.56492	-1.69015
H	16.48318	-0.40300	-4.46731	O	-1.40634	2.74465	0.29156
H	18.08817	-1.04162	-4.87788	O	0.56386	2.54168	-1.47929
C	12.82268	-0.20793	-1.17540	O	0.51177	4.42397	0.77534
C	11.98871	-1.27600	-1.46398	Ti	-3.03099	-2.81920	-3.25923
S	11.87539	1.20900	-0.63841	Ti	-5.57656	-0.65763	-0.20518
C	10.61234	-1.00453	-1.26609	Ti	-2.78350	1.15154	3.88040
H	12.35508	-2.25030	-1.80495	Ti	-4.13565	-4.41647	2.01172
C	10.35332	0.28462	-0.82584	Ti	-3.30407	2.69463	1.01917
H	9.81995	-1.73991	-1.44564	O	0.58998	-6.31713	5.15487
C	9.07849	0.86859	-0.54295	Ti	-0.84970	-5.24444	5.56114
S	7.57007	-0.06908	-0.65791	O	-1.08949	-4.67889	3.71634
C	8.82654	2.18394	-0.15994	Ti	-3.05312	-5.74752	-3.03499

O	-2.61217	-6.43327	-1.44570
Ti	0.95843	1.11901	3.15748
O	-0.58932	-3.70981	6.50121
O	-0.32992	-0.52571	6.57098
O	-1.21809	3.13780	-3.58035
Ti	0.14415	6.23743	0.72798
Ti	0.92466	4.58314	2.82589
O	-1.85761	-4.45351	-3.23057
O	-3.41790	-2.86718	-5.05833
O	-4.83863	-2.06304	-3.01608
O	-6.03630	-2.52062	-0.48863
O	-6.37106	1.10471	-0.56171
O	-3.54118	2.98000	3.57378
O	-2.44588	1.16866	5.68064
O	-0.88100	1.16795	3.64369
Ti	-2.93804	-5.40728	3.96638
Ti	-5.92605	-4.38304	-0.01013
O	-6.04952	-4.44270	1.77648
O	-4.00891	-4.04013	3.98978
O	-4.16626	-4.78579	-0.03227
O	-3.59875	-6.29504	2.60736
Ti	-5.34942	2.75884	-0.50370
O	-5.21466	2.96539	1.25741
O	-3.68085	2.20095	-0.81362
O	-2.92829	4.58271	1.42072
O	-2.44135	-6.08959	5.68325
O	-3.68435	-6.60188	-4.57500
Ti	-5.23735	-5.59439	-4.55962
O	-4.72230	-4.72747	-2.85593
O	1.63771	2.82933	2.61661
O	1.34758	0.99377	4.89163
Ti	-0.53338	1.06603	5.58927
Ti	-2.28574	4.55133	-3.54918
O	-1.53171	6.87406	1.00053
O	1.23349	6.38766	2.22314
O	0.25871	6.65065	-1.05198
O	1.07827	4.99115	4.66033

Ti	-0.48968	4.14864	5.07741
O	-0.86617	3.91884	3.18433
Ti	-5.25789	-2.42713	-4.93832
Ti	-6.65857	-2.29177	-2.56100
Ti	-6.59989	1.13114	-2.60471
Ti	-2.68763	4.58403	3.50700
Ti	-6.48391	-5.40605	-2.28216
O	-6.46500	-6.15322	-0.67145
O	-4.76881	4.63929	-0.89491
Ti	-3.31669	6.36877	1.44763
O	-5.55273	-4.27823	-5.68568
O	-6.73119	-6.40040	-3.82868
O	-0.25788	2.80080	6.25909
Ti	-1.55292	6.25233	-1.51229
O	-2.06959	4.50637	-1.47626
O	-2.97503	4.78185	-5.34825
O	-1.56805	6.30700	-3.31951
Ti	-4.50205	3.90870	-5.00041
O	-4.06546	3.70198	-3.19093
O	-2.07433	4.99770	5.27303
O	-5.35687	-0.76588	-5.75881
O	-7.08357	-2.50807	-4.30232
O	-7.52440	-3.98113	-1.99070
O	-7.28043	-0.62071	-2.13405
Ti	-5.56451	0.85658	-4.93106
O	-4.91234	0.82906	-3.21110
O	-7.25352	1.23947	-4.36784
O	-6.68996	3.13987	-2.12725
O	-3.38979	6.36532	3.25012
Ti	-5.74330	4.66558	-2.74533
Ti	-4.85975	6.43619	-0.81677
O	-5.09189	6.83089	0.95235
O	-3.17734	7.11827	-1.02411
O	-4.79420	2.28642	-5.80895
O	-6.01219	4.85695	-4.59097
O	-6.07259	6.45778	-2.22099

**Table S9.** Cartesian Coordinates of the  $\text{Dhk4-(TiO}_2\text{)}_{38}$  clusters optimized at SSC-DFTB+.

C	21.36024	1.23685	-1.75874	S	7.49452	-0.53283	-0.81183
C	20.57221	0.08995	-1.80988	C	8.83595	1.71727	-0.60327
C	19.16873	0.17907	-1.69151	C	6.60598	0.98334	-0.47250
C	18.55478	1.44472	-1.55198	C	7.48577	2.06256	-0.39968
C	19.37325	2.58163	-1.50742	H	9.65843	2.44023	-0.57787
C	20.76305	2.48912	-1.60089	H	7.14622	3.08556	-0.20012
C	17.04772	1.61691	-1.46803	C	5.19731	1.07999	-0.29210
C	16.32069	0.28355	-1.52484	C	4.26716	0.06640	-0.36139
C	17.00708	-0.94885	-1.66202	H	4.80291	2.08537	-0.06962
C	16.26874	-2.15576	-1.67532	C	2.82820	0.35471	-0.13168
H	16.79819	-3.11402	-1.74925	C	4.61938	-1.29578	-0.64866
C	14.88445	-2.14668	-1.58495	O	2.00412	-0.63010	-0.29754
C	14.17988	-0.92935	-1.46356	O	2.51634	1.56096	0.16770
C	14.92858	0.26713	-1.43128	N	4.84022	-2.40319	-0.87360
H	22.45111	1.15104	-1.84795	Ti	0.15136	-1.09238	0.59574
H	21.04667	-0.88949	-1.94929	O	-1.78118	-1.09549	0.65406
H	18.91247	3.57334	-1.39919	O	-0.20238	-1.43934	-1.33563
H	21.37854	3.39673	-1.56088	O	0.16964	-2.96436	1.13242
H	14.33992	-3.09977	-1.59652	O	0.14813	0.71610	1.20011
H	14.38941	1.21952	-1.32847	Ti	-2.19675	-0.85778	-1.33867
N	18.39507	-0.98718	-1.74684	Ti	-3.53883	-0.90743	1.76584
C	19.05189	-2.25296	-1.89868	H	0.37351	-0.97833	-1.97723
C	19.86044	-2.75263	-0.86515	Ti	-0.46234	-4.75885	0.83508
C	18.88502	-2.98876	-3.08281	Ti	0.89509	-2.71014	3.05119
C	20.50139	-3.98213	-1.02408	Ti	0.56875	2.40333	0.40851
H	19.98533	-2.17540	0.05996	O	-2.86634	-2.82051	-1.39254
C	19.52643	-4.21982	-3.22647	O	-1.70732	0.92131	-1.71203
H	18.25288	-2.59273	-3.88796	O	-2.21389	-1.12974	-3.27768
C	20.33533	-4.71584	-2.20121	O	-3.99769	-0.41462	-0.71297
H	21.13441	-4.37457	-0.21742	O	-5.41972	-0.46878	1.63898
H	19.39838	-4.79576	-4.15235	O	-3.38138	-0.76843	3.64288
C	16.69223	2.33412	-0.14491	O	-3.84975	-2.69547	1.60719
H	17.17066	3.33137	-0.13157	O	-2.87385	0.99666	1.89604
H	15.60152	2.51577	-0.10783	Ti	0.37893	-5.94788	2.87715
C	16.57253	2.50075	-2.64519	Ti	-2.47131	-4.59556	-1.03860
H	15.48598	2.68530	-2.54604	O	-2.27499	-4.67625	0.93265
H	17.06187	3.49058	-2.57883	O	-0.55889	-4.79018	-0.97127
C	17.12016	1.54815	1.06850	O	-0.00968	-6.60720	1.26210
H	16.86183	2.08368	1.99083	O	1.50594	-1.05920	2.36206
H	16.62748	0.56724	1.09547	O	1.69075	-2.80550	4.76237
H	18.20531	1.38133	1.06469	Ti	0.02930	-2.61976	5.44719
C	16.86254	1.87809	-3.98746	O	-0.74770	-2.37966	3.81122
H	16.35444	0.90997	-4.08966	O	1.45457	-4.56984	2.57065
H	16.51903	2.52926	-4.80122	Ti	-1.29644	2.65682	-1.53251
H	17.93950	1.70981	-4.11806	O	-1.32016	2.68259	0.45886
H	20.84056	-5.68291	-2.32050	O	0.57084	2.53597	-1.40100
C	12.73440	-0.91163	-1.35453	O	0.68681	4.23455	0.99324
C	11.86923	-1.99224	-1.43815	Ti	-3.33328	-2.50694	-3.43195
S	11.83254	0.60357	-1.06444	Ti	-5.66321	-0.47690	-0.12460
C	10.50452	-1.65259	-1.27520	Ti	-2.63764	0.88046	3.97266
H	12.20793	-3.01866	-1.61625	Ti	-4.32153	-4.45717	1.74272
C	10.28477	-0.29961	-1.05922	Ti	-3.18920	2.66429	1.25832
H	9.69095	-2.38590	-1.31251	O	0.42431	-6.80394	4.53932
C	9.03532	0.35770	-0.83743	Ti	-0.94706	-5.70358	5.08407

O	-1.22624	-4.98491	3.29952
Ti	-3.48690	-5.43902	-3.42910
O	-3.02197	-6.26500	-1.91517
Ti	1.07024	0.74064	3.10139
O	-0.58017	-4.26210	6.13013
O	-0.16411	-1.10499	6.43059
O	-1.25505	3.37143	-3.37598
Ti	0.40796	6.06091	1.09916
Ti	1.18733	4.21462	3.03094
O	-2.23847	-4.18903	-3.57333
O	-3.78671	-2.39890	-5.21306
O	-5.09284	-1.69103	-3.06146
O	-6.22011	-2.29015	-0.52965
O	-6.38609	1.34110	-0.31538
O	-3.31790	2.76025	3.83504
O	-2.23352	0.74244	5.75400
O	-0.74647	0.82570	3.66198
Ti	-3.09741	-5.64814	3.56401
Ti	-6.18110	-4.18697	-0.19800
O	-6.24188	-4.37958	1.58260
O	-4.10128	-4.24101	3.73587
O	-4.44445	-4.66522	-0.32060
O	-3.85309	-6.39881	2.17226
Ti	-5.28404	2.93756	-0.17264
O	-5.07468	3.00161	1.59218
O	-3.65698	2.33067	-0.59029
O	-2.70729	4.49604	1.78585
O	-2.57194	-6.48376	5.20270
O	-4.21288	-6.14260	-5.00333
Ti	-5.71466	-5.07080	-4.85086
O	-5.09833	-4.36271	-3.10780
O	1.81099	2.45495	2.65757
O	1.51723	0.47066	4.80467
Ti	-0.33224	0.56388	5.57954
Ti	-2.25157	4.82434	-3.19369
O	-1.22403	6.75108	1.48610
O	1.55898	6.04524	2.55448
O	0.47843	6.60677	-0.64693
O	1.42811	4.47248	4.88320

Ti	-0.16214	3.67249	5.29968
O	-0.61795	3.60274	3.41171
Ti	-5.59763	-1.88676	-4.98768
Ti	-6.90390	-1.87405	-2.55321
Ti	-6.68555	1.53556	-2.34030
Ti	-2.39234	4.32442	3.85494
Ti	-6.86822	-5.00432	-2.51751
O	-6.82755	-5.87437	-0.97009
O	-4.62843	4.81428	-0.44460
Ti	-3.01284	6.28992	1.96382
O	-6.00750	-3.65920	-5.86143
O	-7.21799	-5.86312	-4.12434
O	0.04581	2.22906	6.36692
Ti	-1.36568	6.32673	-1.06364
O	-1.96288	4.60797	-1.14039
O	-2.99380	5.22558	-4.94121
O	-1.44302	6.52305	-2.85928
Ti	-4.54627	4.39554	-4.60060
O	-4.05488	4.02850	-2.83121
O	-1.69597	4.57498	5.62088
O	-5.64693	-0.16416	-5.67553
O	-7.40089	-1.93592	-4.28783
O	-7.82877	-3.56155	-2.07788
O	-7.43115	-0.21548	-1.97692
Ti	-5.74856	1.39695	-4.72001
O	-5.03716	1.20708	-3.03424
O	-7.39651	1.80866	-4.06300
O	-6.66299	3.50303	-1.70909
O	-3.02110	6.14925	3.76203
Ti	-5.66785	5.02793	-2.24685
Ti	-4.63261	6.60176	-0.22559
O	-4.78177	6.86582	1.57641
O	-2.92886	7.22333	-0.44712
O	-4.94405	2.85513	-5.51708
O	-5.99427	5.37453	-4.06045
O	-5.89330	6.78642	-1.57471

**Table S10.** Cartesian Coordinates of the DIA3-(TiO<sub>2</sub>)<sub>38</sub> clusters optimized at SSC-DFTB+.

C	14.12422	-0.98822	-1.40062	C	6.53816	0.96360	-0.54679
C	14.80352	-2.22000	-1.58617	C	7.42086	2.03420	-0.41520
C	16.18718	-2.30225	-1.69474	H	9.60116	2.40153	-0.50710
C	16.94449	-1.11505	-1.62755	H	7.08105	3.05426	-0.20166
C	16.27150	0.12958	-1.41226	C	5.12377	1.06497	-0.40958
C	14.87996	0.19529	-1.30279	C	4.18925	0.06152	-0.53327
H	14.22112	-3.14901	-1.63952	H	4.72931	2.06676	-0.17115
H	16.63813	-3.29187	-1.81361	C	2.74717	0.35598	-0.32203
H	14.38370	1.16176	-1.14243	C	4.54052	-1.29531	-0.84566
C	18.52146	0.49204	-1.50409	O	1.91732	-0.62282	-0.49341
C	19.75888	1.14334	-1.46669	O	2.44053	1.56511	-0.03060
C	19.72383	2.52651	-1.25339	N	4.76240	-2.39695	-1.09629
C	18.50467	3.20973	-1.08915	Ti	0.09229	-1.09595	0.46366
C	17.27825	2.54600	-1.12285	O	-1.83514	-1.09923	0.60455
C	17.28631	1.15722	-1.33224	O	-0.33795	-1.42012	-1.45492
H	20.66276	3.09577	-1.20939	O	0.13321	-2.97346	0.98294
H	18.52556	4.29540	-0.92510	O	0.11496	0.70933	1.07857
H	16.33708	3.09440	-0.98673	Ti	-2.33464	-0.84628	-1.36770
C	19.42701	-1.69827	-1.94033	Ti	-3.54583	-0.91463	1.79041
C	21.03116	0.34259	-1.63459	H	0.20751	-0.94549	-2.11309
C	20.73174	-1.13423	-1.89434	Ti	-0.51977	-4.76491	0.70714
C	19.27314	-3.06429	-2.24673	Ti	0.93035	-2.73211	2.87518
C	21.82637	-1.98188	-2.11528	Ti	0.50097	2.40314	0.28337
C	20.38331	-3.87668	-2.46955	O	-3.00732	-2.80793	-1.40643
H	18.27966	-3.50926	-2.33108	O	-1.86324	0.93644	-1.74855
C	21.66778	-3.34018	-2.39281	O	-2.43648	-1.10517	-3.30509
H	22.84298	-1.56732	-2.07212	O	-4.10727	-0.40559	-0.66361
H	20.23769	-4.93873	-2.70554	O	-5.42992	-0.47386	1.74521
H	22.54730	-3.97440	-2.56082	O	-3.31183	-0.78736	3.65999
N	18.31829	-0.87065	-1.69698	O	-3.86606	-2.70109	1.63304
C	21.88401	0.47963	-0.35329	O	-2.87556	0.98835	1.90361
H	22.85092	-0.03819	-0.49862	Ti	0.40030	-5.96950	2.70582
H	22.12363	1.54854	-0.19748	Ti	-2.60389	-4.58657	-1.08173
C	21.83482	0.92155	-2.82105	O	-2.32621	-4.67838	0.87928
H	22.80738	0.40040	-2.89940	O	-0.69114	-4.78667	-1.09416
H	22.06893	1.98198	-2.60910	O	-0.05522	-6.61719	1.10364
C	21.18843	-0.07011	0.86621	O	1.51372	-1.07571	2.17344
H	20.23958	0.45170	1.04662	O	1.79567	-2.83687	4.55156
H	20.96880	-1.13902	0.74494	Ti	0.16380	-2.65492	5.30488
H	21.81636	0.04846	1.75820	O	-0.67959	-2.40620	3.70279
C	21.09107	0.81534	-4.12835	O	1.46523	-4.59096	2.36570
H	21.68343	1.24038	-4.94839	Ti	-1.44312	2.67016	-1.57580
H	20.87434	-0.23272	-4.37332	O	-1.38272	2.68356	0.41562
H	20.13678	1.35600	-4.08216	O	0.42847	2.54599	-1.52339
C	12.67498	-0.96153	-1.30363	O	0.64750	4.23001	0.87476
C	11.80185	-2.02974	-1.43196	Ti	-3.56433	-2.47988	-3.42205
S	11.78204	0.55426	-0.99028	Ti	-5.74709	-0.46939	-0.00656
C	10.43681	-1.68028	-1.28730	Ti	-2.55492	0.85978	3.96840
H	12.13137	-3.05518	-1.63076	Ti	-4.33564	-4.46275	1.77620
C	10.22645	-0.33158	-1.04260	Ti	-3.21684	2.66138	1.29277
H	9.61731	-2.40422	-1.35966	O	0.51268	-6.83623	4.35921
C	8.97488	0.33085	-0.84084	Ti	-0.83176	-5.73572	4.96693
S	7.42860	-0.54913	-0.89229	O	-1.18455	-5.00720	3.19900
C	8.77608	1.68464	-0.57973	Ti	-3.72304	-5.41258	-3.43214



O	-3.19474	-6.24914	-1.94498
Ti	1.11230	0.72078	2.94142
O	-0.41768	-4.30038	6.00379
O	0.01301	-1.14638	6.30488
O	-1.48179	3.39640	-3.41403
Ti	0.37642	6.05607	1.00351
Ti	1.23183	4.19642	2.88970
O	-2.48013	-4.16297	-3.62137
O	-4.09278	-2.35715	-5.18112
O	-5.30511	-1.66412	-2.97108
O	-6.32371	-2.27923	-0.39929
O	-6.47625	1.35025	-0.15263
O	-3.23768	2.74047	3.87298
O	-2.07643	0.71022	5.73016
O	-0.67841	0.80657	3.57778
Ti	-3.04363	-5.66760	3.54126
Ti	-6.27446	-4.17841	-0.08220
O	-6.26092	-4.38199	1.69791
O	-4.03561	-4.25887	3.76065
O	-4.54530	-4.65702	-0.28175
O	-3.85379	-6.40720	2.17445
Ti	-5.36999	2.94640	-0.04530
O	-5.08596	2.99645	1.70958
O	-3.76230	2.34258	-0.53665
O	-2.71197	4.48960	1.81160
O	-2.45166	-6.51315	5.15185
O	-4.51680	-6.10441	-4.97853
Ti	-6.00864	-5.03126	-4.75488
O	-5.31705	-4.33544	-3.03521
O	1.83535	2.43782	2.48019
O	1.63051	0.43673	4.62202
Ti	-0.18477	0.52949	5.47435
Ti	-2.46738	4.84987	-3.17985
O	-1.23701	6.74469	1.46352
O	1.58766	6.02900	2.40936
O	0.37268	6.61134	-0.74101
O	1.55022	4.44145	4.73185
Ti	-0.02175	3.63919	5.20906
O	-0.55694	3.58397	3.34154
Ti	-5.89229	-1.84526	-4.87510
Ti	-7.09361	-1.84882	-2.38756
Ti	-6.86375	1.56027	-2.16070
Ti	-2.30968	4.30385	3.86446
Ti	-7.06151	-4.97908	-2.37488
O	-6.95546	-5.86019	-0.83694
O	-4.72729	4.82553	-0.32954
Ti	-3.00459	6.28307	2.01396
O	-6.34090	-3.61177	-5.74179
O	-7.48122	-5.82646	-3.97089
O	0.23016	2.18809	6.25650
Ti	-1.48800	6.33659	-1.08042
O	-2.09069	4.61922	-1.14231
O	-3.28372	5.26425	-4.89075
O	-1.64199	6.54468	-2.86982
Ti	-4.82169	4.43427	-4.48949
O	-4.25525	4.05619	-2.74465
O	-1.53936	4.54071	5.60140

O	-5.96972	-0.11771	-5.54808
O	-7.66409	-1.89819	-4.09990
O	-8.00052	-3.53821	-1.88483
O	-7.59343	-0.19354	-1.77855
Ti	-6.02989	1.43713	-4.57891
O	-5.24669	1.23600	-2.92668
O	-7.64776	1.84555	-3.84935
O	-6.81296	3.52309	-1.51636
O	-2.93632	6.13064	3.81004
Ti	-5.84090	5.05216	-2.08566
Ti	-4.71618	6.61188	-0.10150
O	-4.78639	6.86719	1.70661
O	-3.02205	7.23114	-0.39264
O	-5.25962	2.90090	-5.39913
O	-6.24459	5.41031	-3.88121
O	-6.03317	6.80714	-1.39423