

Structure-Activity Prediction Networks (SAPNet): a step beyond Nano-QSAR for effective implementation of safe-by-design concept

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Supplementary information

Case study details: Predicting properties of ENMs with SAPNet on example of the phenol degradation efficiency

Table 1S Basic information on the analyzed samples¹

Sample ID	Ionic liquid used during synthesis of TiO ₂	Set (1-training, 2-validation)	Phenol degradation [%]	Phenol degradation (class, 1- high level of degradation, 0 – low level)	ILs decomposition [%]	x _{IL}	x _{TBOT}	BET [m ² ·g ⁻¹]	N [wt%]	C [wt%]
1	triethylsulfonium iodide	1	39	1	75	1	1	186	0.1879	0.2082
2	1-benzyl-3-methylimidazolium chloride	1	44	1	25	1	2	207	0.03	0.248
3	1-butyl-3-methylimidazolium chloride	1	25	0	2	1	2	196	0.01	0.33
4	1-decyl-3-methylimidazolium chloride	2	32	0	7	1	2	218	0.01	0.38
5	3-methyl-1-tetradecylimidazolium chloride	1	61	1	0	1	3	156	0.3167	2.081
6	1,3-didecyl-2-methylimidazolium chloride	1	25	0	5	1	10	211	0.0276	0.327
7	1-methyl-3-octadecylimidazolium chloride	2	59	1	0	1	3	156	0.2206	1.566
8	1-butylpyridinium chloride	1	58	1	50	1	3	215	0.022	0.256

9	1-butyl-1-methylpyrrolidinium chloride	1	49	1	0	1	5	213	0.01	0.575
10	tetrabutylammonium chloride	1	46	1	0	1	2	209	0.018	0.343
11	1-methylimidazolium chloride	1	53	1	80	1	1	208	0.0415	0.24789
12	ethylammonium chloride	1	43	1	29	1	1	188	0.073	0.282
13	hexylammonium iodide	2	42	1	20	1	8	176	0.092	0.4335
14	ethylammonium nitrate	1	88	1	97	1	1	221	0.033	0.325
15	1-butyl-3-methylimidazolium bromide	1	40	1	12	1	2	185	0.132	0.593
16	1-butyl-3-methylimidazolium octylsulfate	2	21	0	4	1	2	202	0.097	0.124
17	2,3,5-triphenyltetrazolium chloride	1	74	1	100	1	10	227	0.0429	0.3097
18	benzyltrimethyltetradecylammonium chloride	1	17	0	95	1	3	189	0.02	0.21
20	tributylmethylammium chloride	2	79	1	12	1	1	188	0.227	1.334
21	1-(2-hydroxyethyl)-3-methylimidazolium chloride	2	53	1	93	1	2	229	0.06	0.77
23	N-butyl-N-methylmorpholinium chloride	1	34	0	14	1	1	222	0.105	0.79

Table 2S Intensity of photoluminescence measured for each sample¹

ID	Sample label	Photoluminescence						
		398 nm	420 nm	440 nm	455 nm	480 nm	502 nm	522 nm
1	TiO2_S222(1:1)	120.806901	148.265969	112.19828	103.721007	82.582204	29.066803	27.725045
2	TiO2_BenMIM(1:2)	55.64021	76.51154	77.94677	67.29667	49.04372	18.02758	17.94582
3	TiO2_BMIM(1:2)	87.53259	111.851856	88.431174	85.326795	63.294931	24.09075	22.560128
4	TiO2_DMIM(1:2)	89.930454	120.353416	99.294083	88.372492	67.36348	24.803	23.62603
5	TiO2_TDMIM(1:3)	5.85292	14.4845	10.243	11.3807	8.05517	2.41108	0.8003
6	TiO2-DDMIM(1:10)	79.509969	96.321431	73.283356	71.829356	58.620954	21.30128	20.435651
7	TiO2_ODMIM(1:3)	10.4347	14.6061	14.162	10.8884	10.4335	4.05983	2.51311
8	TiO2_BPy(1:3)	46.33103	64.23054	57.73754	55.79543	40.04697	16.15598	13.7466
9	TiO2_BMPyr(1:5)	33.0252	54.18158	53.54235	49.10214	38.65786	17.94395	16.52104
10	TiO2_TBA(1:2)	73.63044	106.4344	99.61248	92.41029	66.82512	28.39962	26.00199
11	TiO2_MIM(1:1)	20.2646	35.12861	33.51173	33.11151	27.01868	10.0126	10.55688
12	TiO2_EANCl(1:1)	21.23783	31.90997	33.3914	29.39703	21.46624	8.49272	7.66973
13	TiO2_NH(1:8)	31.49909	42.39091	44.55888	38.7758	25.49047	11.72201	11.10997
14	TiO2_EAN(1:1)	10.64996	16.83355	15.00305	16.75374	11.37264	5.11479	5.0731
15	TiO2_BMIMBr(1:2)	39.76051	61.09788	55.44059	50.48663	33.43227	17.39277	10.9372
16	TiO2_BMIMOct(1:2)	39.06546	67.45093	60.30036	53.94369	36.02839	15.35658	12.85863
17	TiO2_TPTZ(1:10)	22.65812	35.81845	33.57682	31.18517	22.31553	11.57154	7.89987
18	TiO2_BMMTDA(1:3)	114.387227	157.976515	132.089734	116.536015	91.38675	30.184333	31.946446
19	TiO2_[HDPyr][Cl]	-	-	-	-	-	-	-
20	TiO2_TBMA(1:2)	61.05531	85.329757	78.875999	70.094893	57.17931	22.478227	23.061409

21	TiO ₂ _[HOEtMIM][Cl](1:1)	71.982696	106.514643	87.619022	82.208356	68.708386	27.360507	27.061939
22	TiO ₂ _[Chol][Cl](1:1)	-	-	-	-	-	-	-
23	TiO ₂ _[BMMor][Cl](1:2)	77.044007	130.280189	110.094113	101.16303	77.233303	30.234053	34.097075

Table 3S Intensity of UV-Vis absorption spectra measured for each sample¹

ID	Sample label	UV-Vis spectra						
		400 nm	450 nm	500 nm	550 nm	600 nm	650 nm	700 nm
1	TiO ₂ _S222(1:1)	0.102964	0.057026	0.042517	0.03031	0.024616	0.024844	0.016316
2	TiO ₂ _BenMIM(1:2)	0.28102	0.20629	0.16803	0.15256	0.14023	0.13536	0.13145
3	TiO ₂ _BMIM(1:2)	0.162878	0.072237	0.042423	0.032207	0.019723	0.023614	0.027122
4	TiO ₂ _DMIM(1:2)	0.066447	0.003299	-0.012281	-0.016357	-0.017998	-0.012823	-0.01417
5	TiO ₂ _TDMIM(1:3)	0.551625	0.484817	0.407628	0.325104	0.252147	0.192042	0.152395
6	TiO ₂ _DDMIM(1:10)	0.066447	0.003299	-0.012281	-0.032714	-0.035996	-0.012823	-0.02834
7	TiO ₂ _ODMIM(1:3)	0.511383	0.441016	0.360345	0.274148	0.199019	0.134932	0.088231
8	TiO ₂ _BPy(1:3)	0.05585	0.03872	0.01669	0.00946	0.00403	0.00031	-0.01017
9	TiO ₂ _BMPyr(1:5)	0.41802	0.32519	0.25378	0.21379	0.19243	0.16544	0.15026
10	TiO ₂ _TBA(1:2)	0.12508	0.09981	0.06528	0.04563	0.02183	0.01193	0.01291
11	TiO ₂ _MIM(1:1)	0.35606	0.26228	0.20054	0.17569	0.15629	0.14457	0.14192
12	TiO ₂ _EANCI(1:1)	0.20615	0.1157	0.06754	0.03887	0.02038	0.00335	-0.000766
13	TiO ₂ _NH(1:8)	0.25585	0.1774	0.1376	0.10016	0.0801	0.06304	0.04309
14	TiO ₂ _EAN(1:1)	0.62694	0.55078	0.47442	0.41259	0.35272	0.30774	0.27335
15	TiO ₂ _BMIMBr(1:2)	0.130893	0.100997	0.108677	0.119482	0.129889	0.137218	0.145605

16	TiO2_BMIMOct(1:2)	0.174156	0.1121	0.113141	0.121102	0.130851	0.137546	0.145483
17	TiO2_TPTZ(1:10)	0.05926	-0.01621	-0.08531	-0.13223	-0.15646	-0.17212	-0.18169
18	TiO2_BMMTDA(1:3)	0.335323	0.262169	0.235735	0.225635	0.216947	0.203439	0.204123
19	TiO2_[HDPyr][Cl]	0.84807	0.745615	0.6369	0.541075	0.453264	0.372421	0.304178
20	TiO2_TBMA(1:2)	0.522323	0.42237	0.34116	0.29196	0.245143	0.245189	0.220124
21	TiO2_[HOEtMIM][Cl](1:1)	0.45386	0.310725	0.200744	0.122206	0.070737	0.035121	0.009269
22	TiO2_[Chol][Cl](1:1)	0.548641	0.391245	0.250955	0.139436	0.065164	0.013736	-0.018934
23	TiO2_[BMMor][Cl](1:2)	0.215382	0.113159	0.062559	0.032647	0.014446	0.001856	-0.006658

Table 4S Loadings values of PCs

Variable	PC1	PC2	PC3	PC4	PC5	PC6	PC7
ILs decomposition [%]	-0.359	0.112	-0.661	0.143	0.011	0.599	-0.206
molar ratio (IL:TBOT)	-0.088	0.575	0.284	-0.692	-0.061	0.314	-0.019
BET [m ² ·g ⁻¹]	-0.486	-0.086	0.179	0.130	-0.778	0.015	0.318
N [wt%]	0.510	0.066	-0.383	-0.108	-0.130	0.150	0.733
C [wt%]	0.473	0.315	-0.203	0.098	-0.573	-0.188	-0.512
Type of cation	-0.373	0.458	-0.389	-0.053	0.140	-0.670	0.169
Type of anion	-0.063	-0.581	-0.332	-0.678	-0.158	-0.190	-0.166

References:

1. Rybińska-Fryca, A. *et al.* How thermal stability of ionic liquids leads to more efficient TiO₂-based nanophotocatalysts: theoretical and

experimental studies. *J. Colloid Interface Sci.* (2020) doi:10.1016/j.jcis.2020.03.079.