Electronic Supplementary Information

An Integrated Experimental and Theoretical Approach to Probe Cr(VI) Uptake using Decorated Halloysite Nanotubes for Efficient Water Treatment

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Cartesian coordinates

$HCrO_4^-$:

Cr	-1.411592	0.597902	-0.059386
O	-0.821598	1.461145	1.435790
O	-2.996830	0.634967	0.004791
O	-0.849249	-0.891073	-0.025363
O	-0.849234	1.371835	-1.331868
H	0.140353	1.462129	1.437560

H1:

C	-0.705069	0.393824	-0.006975
C	0.664288	0.611746	-0.100754
C	1.189091	1.903615	-0.071836
C	0.314618	2.995923	0.042292
C	-1.057224	2.780955	0.147573
C	-1.563859	1.484549	0.121700
H	-1.113487	-0.611071	-0.014419
H	1.345209	-0.228337	-0.184343
H	-1.733204	3.622648	0.247927
C	2.663504	2.099046	-0.114143
N	3.289636	1.646515	-1.147184
N	3.260666	2.707732	0.951114
H	4.214571	3.012992	0.834586
H	2.683668	3.212779	1.604532
O	4.671261	1.906347	-1.004678
H	5.043273	1.533288	-1.807909
C	0.825032	4.394914	0.009168
N	0.513318	5.157586	1.000716
N	1.545067	4.791212	-1.081608
O	1.063858	6.440480	0.792347
H	2.053089	5.658688	-0.997824
H	1.939761	4.080708	-1.678325
H	0.791064	6.920793	1.578363
O	-2.911240	1.304465	0.255753
Si	-3.905304	0.710408	-0.920532
O	-3.783799	1.623189	-2.285748
H	-3.793284	2.578872	-2.203018
O	-5.364876	0.731768	-0.189387
H	-6.043752	0.154846	-0.543816
O	-3.534267	-0.816170	-1.400518
H	-3.073769	-0.896057	-2.239328

H2:

C	-0.674339	0.381195	-0.122065
C	0.691143	0.604077	-0.257149
C	1.224689	1.888111	-0.150725
C	0.360038	2.971118	0.081463
C	-1.006712	2.749713	0.230342
C	-1.520706	1.459906	0.129039
H	-1.087487	-0.619678	-0.188479
H	1.364296	-0.227949	-0.433868
H	-1.672919	3.582911	0.424916
C	2.697090	2.084598	-0.233542
N	3.320497	1.662159	-1.276374
N	3.327764	2.671220	0.847855
H	2.729680	3.134173	1.517821
H	4.165705	3.191166	0.613483
C	0.877466	4.367175	0.126201
N	0.608619	5.092229	1.153278
N	1.581509	4.826530	-0.971917
H	1.903710	4.122664	-1.621809
H	2.278025	5.530214	-0.753506
O	-2.862972	1.271321	0.309452
Si	-3.908270	0.777874	-0.867924
O	-3.834194	1.798771	-2.158605
H	-3.804029	2.743274	-1.993711
O	-5.338473	0.745395	-0.080586
H	-6.031626	0.196535	-0.451545
O	-3.576086	-0.707831	-1.485721
H	-3.129373	-0.721913	-2.335604
N	1.149755	6.391124	1.077649
H	0.812762	6.878830	0.245419
H	0.817550	6.894556	1.890496
N	4.710431	1.898855	-1.229763
H	5.127011	1.454573	-0.409212
H	5.108098	1.464458	-2.053029

H3:

C	1.795798	-1.992482	-1.098646
C	0.433977	-2.000472	-0.819444
C	-0.198289	-0.894360	-0.250574
C	0.566319	0.241851	0.061265
C	1.930048	0.254760	-0.224024
C	2.541998	-0.855619	-0.797550
H	2.281929	-2.849624	-1.552388
H	-0.161574	-2.879607	-1.042685
H	2.518412	1.139263	-0.005530

C	-1.664950	-0.975652	0.010499
N	-2.047856	-1.915853	0.823271
N	-2.497912	-0.098930	-0.606174
H	-3.485475	-0.186548	-0.361033
C	-0.011981	1.463891	0.698473
N	0.058169	2.553997	0.008458
N	-0.578603	1.388251	1.940676
H	-0.712764	2.303993	2.353716
O	3.878531	-0.797631	-1.087162
Si	5.032294	-1.668865	-0.292233
O	4.970493	-1.356806	1.323840
H	4.834085	-0.451821	1.611161
O	6.407259	-1.208137	-1.044220
H	7.165548	-1.789510	-0.964494
O	4.850699	-3.297245	-0.415841
H	4.440072	-3.733755	0.334557
N	-0.505602	3.672548	0.676881
H	-1.517812	3.540845	0.723317
N	-3.470810	-1.943364	0.964832
H	-3.637287	-2.375713	1.866163
C	-0.486684	0.263551	2.856838
C	-1.853886	-0.102392	3.434950
H	0.220174	0.478433	3.667605
H	-0.100370	-0.602174	2.316724
H	-2.144022	0.628633	4.199446
H	-2.593693	-0.049523	2.623581
C	-0.225926	4.889769	-0.078701
C	1.243217	5.278178	0.038691
H	-0.850643	5.684343	0.348121
H	-0.481398	4.784230	-1.142662
H	1.516402	5.296833	1.105815
H	1.843254	4.497837	-0.438166
C	-2.154753	0.784126	-1.703275
C	-3.159621	0.725885	-2.849710
H	-1.160125	0.520016	-2.074761
H	-2.079702	1.823930	-1.364150
H	-2.800231	1.423191	-3.620572
H	-4.130104	1.100327	-2.501819
C	-4.126655	-2.753290	-0.072915
C	-5.529905	-2.234209	-0.369409
H	-4.165322	-3.818734	0.197680
H	-3.528113	-2.679735	-0.986944
H	-6.062793	-2.994633	-0.963934
H	-6.079840	-2.114156	0.571291
N	1.482807	6.537730	-0.661293
H	1.104028	7.323457	-0.143305
H	2.473608	6.705787	-0.787588

N	-1.754842	-1.416276	4.061536
H	-2.594499	-1.641873	4.582019
H	-1.631593	-2.117445	3.334048
N	-3.349798	-0.638838	-3.349562
H	-3.762037	-0.627409	-4.276337
H	-2.457756	-1.118603	-3.427306
N	-5.448749	-0.935001	-1.032117
H	-4.999337	-1.037493	-1.943715
H	-6.368839	-0.531152	-1.163871

H4:

C	3.417852	-1.440812	-1.792066
C	2.182383	-1.694890	-1.207895
C	1.475163	-0.693806	-0.542373
C	2.033582	0.592062	-0.450935
C	3.267483	0.851077	-1.042875
C	3.957284	-0.159745	-1.706444
H	3.959322	-2.216899	-2.322501
H	1.745015	-2.685974	-1.268647
H	3.693430	1.847447	-0.992995
C	0.157422	-1.026020	0.068718
N	0.147837	-2.015247	0.906844
N	-0.916236	-0.255854	-0.243717
H	-1.753869	-0.429155	0.303928
C	1.376918	1.711652	0.290771
N	0.970004	2.719534	-0.403914
N	1.242712	1.632981	1.654864
H	1.120176	2.552219	2.068449
O	5.157198	0.135649	-2.295655
Si	6.609378	-0.423314	-1.747515
O	6.820638	-0.002930	-0.168664
H	6.555045	0.875789	0.109749
O	7.669091	0.239689	-2.798957
H	8.527712	-0.179772	-2.877320
O	6.757076	-2.059773	-1.772792
H	6.604384	-2.509233	-0.938038
N	0.378856	3.733535	0.384613
H	-0.450830	3.349117	0.844566
N	-1.153496	-2.332501	1.402852
H	-0.971518	-2.870880	2.246438
C	1.922572	0.650851	2.485286
C	1.276283	0.612051	3.868168
H	2.997443	0.856507	2.585171
H	1.811908	-0.328207	2.019075
H	1.481540	1.552806	4.394343
H	0.183346	0.540916	3.723861

C	-0.003338	4.861299	-0.465660
C	-0.765428	5.935479	0.321657
H	-0.612705	4.540223	-1.323551
H	0.925812	5.272856	-0.867702
H	-0.513814	5.827749	1.392698
H	-0.414771	6.922948	0.009421
C	-1.165292	0.348461	-1.539039
C	-2.185665	1.468716	-1.369970
H	-1.535661	-0.405365	-2.251461
H	-0.242452	0.768578	-1.945561
H	-2.415293	1.896257	-2.361359
H	-1.702628	2.253325	-0.781945
C	-1.870450	-3.203709	0.465519
C	-3.168767	-3.704576	1.090973
H	-1.259820	-4.064539	0.156300
H	-2.097873	-2.626355	-0.438166
H	-2.927628	-4.360102	1.935803
H	-3.730631	-2.846386	1.496538
N	-2.205923	5.902786	0.074771
H	-2.629234	6.746009	0.448232
N	1.806252	-0.484512	4.664451
H	1.604801	-0.325013	5.641762
N	-3.372162	1.016666	-0.659073
H	-3.806620	1.796542	-0.164619
N	-3.942943	-4.468291	0.117728
H	-4.462972	-5.204433	0.579903
C	-4.839829	-3.662251	-0.694231
C	-5.323535	-4.438528	-1.913976
H	-4.299251	-2.775551	-1.042662
H	-5.709742	-3.284294	-0.123941
H	-4.465549	-4.627354	-2.565188
H	-5.702007	-5.423468	-1.596220
C	-4.374898	0.386446	-1.504340
C	-5.543157	-0.111539	-0.661998
H	-3.921227	-0.466438	-2.029126
H	-4.763282	1.064959	-2.284055
H	-5.155115	-0.835810	0.073803
H	-5.942537	0.733945	-0.088438
C	-2.887911	4.735384	0.602769
C	-4.347744	4.708813	0.169232
H	-2.819017	4.656870	1.706337
H	-2.413078	3.839758	0.193648
H	-4.857726	5.617400	0.529893
H	-4.378931	4.732444	-0.923857
C	1.335687	-1.806762	4.246286
C	2.412055	-2.630622	3.533363
H	0.477929	-1.702047	3.566088

H	0.979541	-2.375118	5.112631
H	2.969677	-1.972558	2.849884
H	3.133164	-2.994904	4.273328
N	1.786583	-3.766626	2.860236
H	1.379657	-3.434634	1.985189
H	2.471181	-4.479174	2.635999
N	-4.982530	3.470563	0.622146
H	-5.063969	3.449055	1.633928
H	-5.919984	3.386070	0.244522
N	-6.604609	-0.629826	-1.515544
H	-6.312321	-1.471376	-2.013189
H	-7.418813	-0.877019	-0.964531
N	-6.314196	-3.653196	-2.652074
H	-6.391711	-3.964653	-3.612953
H	-7.234888	-3.742029	-2.234626

Complex H1 – $HCrO_4^-$:

C	1.071520	-1.431151	-0.991012
C	-0.199889	-1.878045	-0.649419
C	-1.156068	-1.004750	-0.130376
C	-0.819455	0.344496	0.051204
C	0.449920	0.801802	-0.303527
C	1.389926	-0.086378	-0.814606
H	1.815140	-2.106846	-1.401429
H	-0.468965	-2.920630	-0.780270
H	0.700761	1.851078	-0.184422
C	-2.517734	-1.518744	0.208285
N	-2.546681	-2.409942	1.141819
N	-3.568917	-1.028025	-0.519436
H	-4.484734	-1.069861	-0.080880
H	-3.417404	-0.142334	-0.980453
O	-3.824890	-2.912776	1.427015
H	-4.437773	-2.162625	1.597659
C	-1.791775	1.299620	0.659125
N	-2.036815	2.361650	-0.036294
N	-2.289939	1.002105	1.886307
O	-2.990828	3.159818	0.648061
H	-3.141785	1.459674	2.208697
H	-2.203805	0.042838	2.192579
H	-3.066019	3.930552	0.079159
O	2.643939	0.379188	-1.140972
Si	3.923537	0.161802	-0.123575
O	3.477461	0.550563	1.411393
H	2.602187	0.921758	1.550814
O	5.117689	1.096092	-0.738533
H	5.999771	0.722827	-0.697586

O	4.504940	-1.382090	-0.084592
H	4.128336	-1.947755	0.593794
Cr	-5.909128	0.781150	1.692187
O	-7.449346	1.046904	1.890450
O	-5.602611	-0.799237	1.592656
O	-5.045899	1.470548	2.837028
O	-5.374131	1.518228	0.144017
H	-4.647875	2.141758	0.301700

Complex H2 – $HCrO_4^-$:

C	-2.950797	1.493580	-0.931931
C	-1.679222	2.037768	-0.785860
C	-0.576239	1.232251	-0.499816
C	-0.763291	-0.152378	-0.355491
C	-2.033479	-0.705390	-0.520567
C	-3.119599	0.117114	-0.799507
H	-3.808741	2.117353	-1.162719
H	-1.523276	3.105909	-0.894639
H	-2.169710	-1.779304	-0.436946
C	0.780553	1.843809	-0.374220
N	0.929037	2.729068	0.547538
N	1.734606	1.430296	-1.278216
H	2.706804	1.464991	-0.979664
H	1.540581	0.567789	-1.766856
C	0.382175	-1.037135	0.010300
N	0.605199	-2.050242	-0.752438
N	1.065054	-0.726782	1.162252
H	2.067454	-0.940175	1.224187
H	0.858533	0.185258	1.546587
O	-4.371947	-0.445086	-0.934806
Si	-5.440353	-0.424407	0.319705
O	-4.661130	-0.835771	1.709833
H	-3.732095	-1.075243	1.646814
O	-6.635968	-1.456229	-0.110622
H	-7.524252	-1.176630	0.117181
O	-6.161745	1.039121	0.574578
H	-5.705553	1.621528	1.186563
Cr	4.602079	-0.423981	0.165270
O	6.157013	-0.686259	0.130205
O	4.284173	1.149131	0.239517
O	3.900846	-1.214951	1.369713
O	3.845576	-1.046899	-1.325089
H	3.185467	-1.737659	-1.105509
N	2.193450	3.325685	0.631712
H	2.236122	3.792095	1.528060
H	2.965638	2.652919	0.583622

N	1.743641	-2.803025	-0.421582
H	1.886426	-2.916535	0.583568
H	1.647132	-3.712391	-0.854214

Complex H3 – $HCrO_4^-$:

C	-4.040678	1.259881	-0.758946
C	-2.841128	1.948745	-0.629132
C	-1.617083	1.283311	-0.516951
C	-1.606286	-0.122933	-0.535185
C	-2.810879	-0.813765	-0.679786
C	-4.016599	-0.130633	-0.778896
H	-4.986522	1.784026	-0.850370
H	-2.837928	3.032971	-0.601984
H	-2.794442	-1.897517	-0.736963
C	-0.405994	2.141506	-0.332512
N	-0.461346	2.957822	0.687020
N	0.627287	2.095299	-1.193376
H	1.456790	2.594731	-0.878173
C	-0.368522	-0.962261	-0.450259
N	-0.173739	-1.739153	-1.476947
N	0.440996	-0.887092	0.626009
H	1.306897	-1.425523	0.560889
O	-5.187530	-0.844334	-0.906202
Si	-6.150747	-1.146236	0.395234
O	-5.242685	-1.698050	1.651372
H	-4.339291	-1.974845	1.478014
O	-7.272059	-2.199566	-0.164542
H	-8.135391	-2.146938	0.248860
O	-6.970203	0.168667	0.963071
H	-6.517885	0.664805	1.649829
N	1.019054	-2.511581	-1.317413
H	1.387572	-2.647431	-2.252290
N	0.704013	3.793185	0.745140
H	0.839069	3.994126	1.730671
C	0.202422	-0.199229	1.877913
C	1.355159	0.737737	2.229160
H	0.072142	-0.929149	2.687090
H	-0.723377	0.377958	1.804914
H	2.237573	0.145359	2.486233
H	1.616534	1.330771	1.343813
C	0.751457	-3.815439	-0.718531
C	2.059110	-4.580447	-0.562964
H	0.022707	-4.400575	-1.310279
H	0.313590	-3.662707	0.273612
H	2.598570	-4.581248	-1.524522
H	2.686132	-4.038978	0.148981

C	0.829132	1.309297	-2.393624
C	2.164791	0.569162	-2.283321
H	0.854820	1.987934	-3.258942
H	0.012221	0.601341	-2.540205
H	2.340688	0.013803	-3.214376
H	2.094971	-0.173913	-1.484978
C	0.488895	5.050892	0.034870
C	1.759785	5.889680	0.077019
H	-0.362076	5.620278	0.450746
H	0.245636	4.823888	-1.007783
H	2.105310	5.969993	1.122682
H	2.543559	5.363861	-0.476001
N	1.797353	-5.928225	-0.049256
H	1.420247	-6.527074	-0.776637
H	2.656386	-6.353292	0.279884
N	0.958736	1.549379	3.382480
H	1.743994	2.103268	3.706307
H	0.222899	2.189669	3.092249
N	3.244064	1.510486	-1.976875
H	3.795639	1.164163	-1.191694
H	3.864292	1.635847	-2.766440
N	1.531728	7.188530	-0.556467
H	0.886224	7.748318	-0.008838
H	2.397228	7.710115	-0.633928
Cr	4.366340	-1.401715	0.513513
O	5.845313	-1.926185	1.407958
O	3.115187	-2.001811	1.298999
O	4.456433	-1.969758	-0.962584
O	4.308322	0.192004	0.480608
H	6.632801	-1.770863	0.877252

Complex H4 – $HCrO_4^-$:

C	-4.252652	-2.028137	1.889008
C	-2.959868	-1.937958	1.385254
C	-2.537022	-0.818869	0.667823
C	-3.441408	0.234016	0.449428
C	-4.734432	0.151027	0.962893
C	-5.138866	-0.977060	1.671099
H	-4.575444	-2.893458	2.458774
H	-2.252776	-2.744867	1.546687
H	-5.429484	0.971898	0.816987
C	-1.147786	-0.787079	0.127511
N	-0.802183	-1.788226	-0.619140
N	-0.380145	0.302820	0.391414
H	0.502331	0.348281	-0.111444
C	-3.095889	1.442852	-0.360449

N	-3.042070	2.574200	0.256633
N	-2.865526	1.302843	-1.706161
H	-2.967085	2.185340	-2.196959
O	-6.422395	-1.031610	2.156065
Si	-7.584968	-1.965972	1.450735
O	-7.547213	-1.745504	-0.180383
H	-7.070128	-0.988439	-0.528013
O	-8.971685	-1.502036	2.181880
H	-9.622133	-2.190608	2.330264
O	-7.413031	-3.584784	1.701899
H	-6.949298	-4.065477	1.012049
N	-2.711712	3.652411	-0.599259
H	-1.771100	3.492250	-0.970080
N	0.548522	-1.728928	-1.065905
H	0.587694	-2.383356	-1.842289
C	-3.195472	0.107573	-2.463403
C	-2.445458	0.103799	-3.792190
H	-4.275128	0.013989	-2.651618
H	-2.879926	-0.759662	-1.884544
H	-2.807893	0.928398	-4.419415
H	-1.379372	0.289851	-3.574489
C	-2.733571	4.905884	0.155099
C	-2.268349	6.092791	-0.700417
H	-2.115263	4.848957	1.063195
H	-3.767423	5.052903	0.478282
H	-2.397636	5.824496	-1.765388
H	-2.919193	6.950206	-0.505898
C	-0.365425	1.014360	1.657078
C	0.291389	2.374816	1.443809
H	0.185463	0.438171	2.416403
H	-1.385730	1.163036	2.019972
H	0.359494	2.893889	2.416773
H	-0.383151	2.958672	0.810685
C	1.489205	-2.211936	-0.041673
C	2.899097	-2.285394	-0.621306
H	1.199376	-3.201484	0.340451
H	1.469822	-1.514915	0.802772
H	2.891005	-2.977462	-1.473600
H	3.175448	-1.289733	-1.014049
N	-0.905424	6.517340	-0.387513
H	-0.723264	7.412030	-0.830460
N	-2.660712	-1.146355	-4.509369
H	-2.396194	-1.025383	-5.477525
N	1.574128	2.248452	0.775883
H	1.781276	3.087502	0.235312
N	3.851349	-2.785986	0.357843
H	4.671136	-3.109286	-0.153216

C	4.340729	-1.740862	1.253326
C	5.304521	-2.313809	2.283214
H	3.498308	-1.268045	1.774761
H	4.866606	-0.952694	0.692088
H	4.748837	-2.936691	2.993735
H	6.028240	-2.962444	1.766516
C	2.695762	1.986407	1.669297
C	3.984140	1.796021	0.879909
H	2.493701	1.071408	2.243183
H	2.842051	2.797045	2.406104
H	3.852959	0.925491	0.216742
H	4.127850	2.666801	0.226002
C	0.126285	5.566106	-0.763726
C	1.500091	6.011864	-0.277463
H	0.155889	5.372717	-1.854526
H	-0.088061	4.609524	-0.280575
H	1.743692	6.999717	-0.705052
H	1.451774	6.134318	0.808453
C	-1.951894	-2.290584	-3.928965
C	-2.865662	-3.233206	-3.139442
H	-1.157967	-1.940307	-3.253688
H	-1.459499	-2.867052	-4.719239
H	-3.580043	-2.634232	-2.553434
H	-3.461532	-3.828570	-3.840878
N	-2.042008	-4.120487	-2.325388
H	-1.663046	-3.583587	-1.543239
H	-2.591051	-4.882416	-1.944762
N	2.489490	4.982911	-0.580802
H	2.698824	4.935948	-1.572095
H	3.361705	5.140599	-0.089173
N	5.125658	1.698200	1.777391
H	5.008521	0.908440	2.412954
H	5.959641	1.462279	1.241868
N	5.954813	-1.217063	3.005281
H	6.517595	-1.593711	3.760689
H	6.608692	-0.767270	2.361488
Cr	7.834804	-1.415202	-0.352762
O	6.446952	-2.260797	-1.181615
O	8.414088	-2.456102	0.688888
O	7.262021	-0.116471	0.390638
O	8.895486	-1.011846	-1.456649
H	6.197303	-1.781990	-1.977933