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Title: Assessment of halloysite clay nanotubes as adsorbents for removing tetracycline hydrochloride from contaminated aqueous systems via experimental study and SQM calculations.

Author(s): Mariana R. L. Silva, Aisha V. S. Pereira, Anne B. F. Câmara, Heloise O. M. A. Moura, Sérgio R. B. Silva, Miguel A. F. de Souza, Luiz C. Bertolino, Daniel Ballesteros-Plata, Enrique Rodríguez-Castellón, Luciene S. de Carvalho

SUPPLEMENTARY MATERIAL ES2

Semi-empirical computational calculations

The software employed for data analysis and image generation included **OriginPro 2019b**, **Design of Experiments**, **Lucid Charts**, and **Microsoft Excel**. Semi-empirical computational calculations were performed using the **GFN1-xTB** method.

The script of the xTB software as follow:

```
xtb dock halo.xyz tetrazw.xyz --gfn 1 --etemp 1000.0 --input xtb.inp  
xtb dock halo.xyz tetra.xyz --gfn 1 --etemp 1000.0 --input xtb.inp
```

XYZ coordinates for optimized structures of the system: halloysite + tetracycline (neutra form)

584

-1687.56642361400554

O	-10.22315309360982	-6.99573673381078	2.81315804632234
O	-15.10335354638048	-8.58993688171602	2.86865805147145
O	-12.27035328354304	-9.17613693610192	2.82625804753771
O	-7.36015282798908	-7.65323679481173	2.76025804141443
O	-9.27685300581488	-9.88123700151899	2.81965804692542

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Al	-13.48875339658260	-8.07653683408425	1.90855796239620
Al	-8.59875294290276	-6.53223669080863	1.62625793620523
Al	-7.69195285877253	-9.34133695142870	1.92425796385276
Al	-11.48705321087076	-5.89973663212714	1.62935793649285
Si	-13.94765343915796	-9.91973700509079	-1.38674234333196
Si	-9.01195298123824	-8.39383686352241	-1.44724234894505
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Si	0.59744791029364	-13.13763730363827	-1.44614234884296
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Si	4.59044828075247	-8.75483689701493	-1.54144235768470
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O	-2.17825234722763	1.75496407805344	2.50405801764495
Al	-2.59455238585072	0.05536392036955	1.39815791504279
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Si	2.79884811453310	-3.08593637107105	-1.70034237242695
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O	-1.44685227937049	1.78066408043781	-2.52414244885669
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O	-1.83685231555354	3.35206422622769	-0.02044221657075
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O	4.49484827188299	-2.32003630001309	2.61435802787822
O	7.36184853787485	-2.97833636108823	2.57065802382389
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Al	6.09804842062318	-1.86303625761397	1.40595791576645

Al	10.97394887299486	-0.28553611125816	1.33865790952256
Al	11.83644895301508	-3.12403637460585	1.38385791371607
Al	8.11474860772668	0.34066394683884	1.30555790645163
Si	5.69814838352162	-3.72243643012363	-1.69104237156413
Si	10.59484883782308	-2.16133628528938	-1.74384237646273
Si	11.51054892277905	-4.99293654799691	-1.59454236261114
Si	7.69544856882526	-1.52343622610688	-1.74274237636070
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O	9.15114870388083	-1.98473626890494	-2.44664244166647
O	6.70714847713368	-2.65223633083363	-2.44524244153658
O	11.64654893539671	-1.08603618552620	-2.43514244059952
O	11.09334888407244	-3.61933642055833	-2.37124243467108
O	7.27164852950634	-0.13543609733230	-2.50904244745575
O	12.63834902741301	0.19176393302434	0.04135778916285
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O	6.85354849071625	1.43926404876372	-0.02104221662642
O	10.66614884443808	-2.04013627404479	0.06525779138025
O	-6.89425278476426	8.09846466658475	2.40675800861776
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Al	-10.19665309115123	6.98556456333315	1.39845791507063
Al	-5.27955263495713	8.55056470852925	1.22355789884392
Al	-4.37065255063206	5.71896444582172	1.31205790705469
Al	-8.16705290285091	9.19176476801790	1.23265789968818
Si	-10.61325312980217	5.13666439179763	-1.77974237979343
Si	-5.69105267313489	6.69536453640925	-1.87994238908970
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H	11.76904894669918	-10.38013704785584	-1.80184238190980
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C	4.33625688499320	-7.20387615316560	7.18170754276931
C	3.83565355323812	-5.89437823498686	7.25251962208523
C	2.68429299022294	-5.57470175697314	6.51501759919136
C	2.04538641729929	-6.54353179431889	5.75277887374387
C	2.54902821959139	-7.83773211561331	5.69805815573094
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H	1.16129363778598	-6.30903134695634	5.17278690657276
H	2.05366663791554	-8.58189343201449	5.08241439374066
O	5.47749295690177	-7.52336299754519	7.83645446444444
H	5.71726119796063	-8.44670896223662	7.68673327742132
C	2.24260063166937	-4.11311542315322	6.54051447972752

O	1.75738687113529	-3.75465080218531	7.83210226748242
H	0.98761663053106	-4.29666210884450	8.04521474021466
C	1.15942785256858	-3.78607779632827	5.51688211915450
H	0.28243982971693	-4.41098805139931	5.68393665039491
H	0.85352362108364	-2.74662265770253	5.62526367093884
H	1.53253273570067	-3.94533984493608	4.51021809409297
C	4.50692042610576	-4.85129077140775	8.10528640889874
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C	3.55991211054004	-3.31682834422894	6.32108821762206
H	4.10707465806638	-3.80359259391367	5.49892750514602
C	3.30818176487528	-1.86006335321206	5.92903929663785
H	3.07131735374332	-1.80176952510666	4.86344950198653
H	2.44310141288587	-1.48664518164266	6.48293962720375
C	4.53057868894168	-0.99242067624974	6.24800851342723
H	5.42709825122403	-1.44117577684744	5.80454846440203
C	4.68627412127548	-0.96856879583692	7.77113279336836
C	4.79834562450560	-2.39570037339336	8.29830440721795
C	4.34995690610461	-3.46696000066250	7.60512997667087
O	5.42804889562694	-2.48376017019738	9.46762798307559
H	5.69203039118682	-1.58811347513139	9.74451128170789
O	5.85504273654918	-0.28248457266626	8.16818867087954
H	5.85370391052495	0.55981281214340	7.61838565400937
C	4.35064935188312	0.43734180435263	5.72563760714718
H	4.33548671150124	0.45012991898985	4.62907907455417
C	3.02347515423165	0.93592108743497	6.25011426046806
C	2.70479471090574	0.66367453015728	7.61651325973972
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C	6.66357989178827	1.07093185875451	5.41491959565661
H	7.45755348153022	1.71662476399844	5.79083328511599
H	6.96231889843718	0.03117782649835	5.54044713627566
H	6.48540047194306	1.27729457109956	4.35713450507904
C	5.05450735226229	2.74434681348453	5.98050075661317
H	5.90774953376392	3.37399913745424	6.23144116974410
H	4.76716195792881	2.91244344354375	4.93570867439883
H	4.22341398437076	2.99282205728764	6.63939149960657

O	2.24240030289462	1.53715230570804	5.48670528270681
H	1.20769102266614	1.88784458236260	6.37490151136183
C	3.50869154215300	-0.20817617283940	8.45592360236792
O	3.32662158458748	-0.34619039347523	9.65322901667444
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H	1.63047131536020	0.50497895494386	9.98885570901543
O	0.71602958484680	1.91384073728888	7.32233539500562

XYZ coordinates for optimized structures of the system: halloysite + tetracycline (zwitterionic form)

584

-1687.57302925811041

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O	-13.09465336004907	-6.40613667913615	2.77335804258704
Al	-13.48875339654460	-8.07653683412993	1.90855796234222
Al	-8.59875294289808	-6.53223669084145	1.62625793622698
Al	-7.69195285877965	-9.34133695143220	1.92425796389235
Al	-11.48705321085715	-5.89973663213368	1.62935793650215
Si	-13.94765343918439	-9.91973700533995	-1.38674234333951
Si	-9.01195298119542	-8.39383686353703	-1.44724234893587
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O	-0.05260120530349	-2.54249394027267	7.36581458773258
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O	1.09975883955607	1.49995980252991	9.53850018076495
C	0.95309157445451	-1.31201986299510	9.82117875218778
N	0.32425069806170	-2.51118777576245	10.01468269791824
H	0.73625522902549	-3.06458815010550	10.74727599030350
H	-0.00839409737317	-3.00464578195182	9.20077583452296
O	1.70477467172099	-0.86988036384163	10.66362068429850
H	-1.86697961957938	0.12891845628021	7.05322691569916