

Supplementary materials

Removal of 17 β -estradiol by Activated Charcoal Supported Titanate Nanotubes (TNTs@AC) through Initial Adsorption and Subsequent Photo-Degradation: Intermediates, DFT calculation, and Mechanisms

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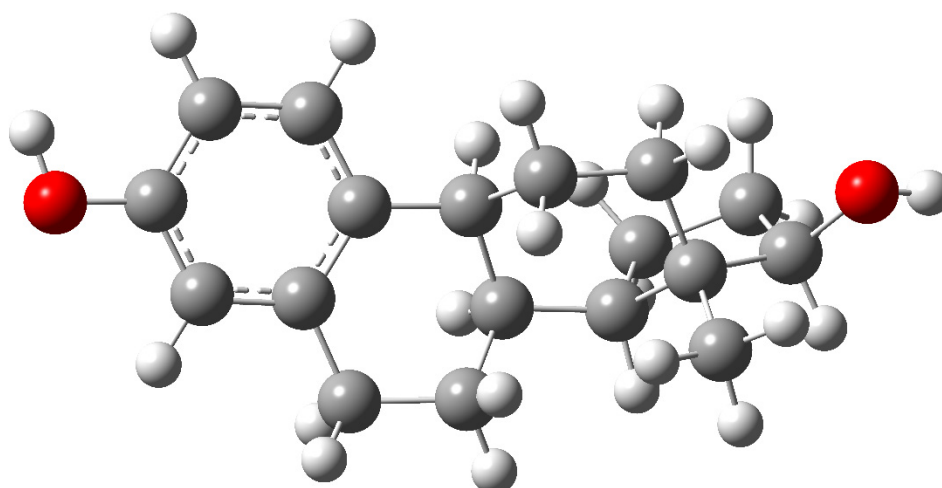
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Figures:

Figure S1. Optimized geometry coordinates and structure of E2.



Electronic state: 1-A

Tables:

Table S1. Cartesian coordinates (Angstroms).

Cartesian coordinates (Angstroms)			
	X	Y	Z
C	-1.78165000	-0.40329900	0.20845700
C	-2.47058100	0.81318300	0.02710800
C	-3.86940100	0.80952600	-0.09377900
C	-4.58928900	-0.38166400	-0.02747800
C	-3.92292600	-1.59674600	0.16218300
C	-2.53271000	-1.58925600	0.27637900
H	-4.40457200	1.74514200	-0.23652400
H	-4.48455400	-2.52552600	0.22125300
H	-2.01551000	-2.53432200	0.42635100
C	-1.73341100	2.13928600	0.00364500
H	-1.86947000	2.62788500	0.97981200
H	-2.19856600	2.80361700	-0.73413100
C	-0.23469900	1.98711700	-0.27267900
H	0.26998100	2.94443400	-0.09547000
H	-0.08223500	1.74008000	-1.32912400
C	0.36964700	0.90027300	0.63397600
H	0.07350200	1.16422300	1.66165700
C	-0.26241800	-0.47596600	0.31441100
H	-0.02872900	-1.15768200	1.14417700
C	0.36975900	-1.10120500	-0.95104200
H	-0.07675000	-2.08707800	-1.12660900
H	0.12394000	-0.49043400	-1.82865700
C	1.91557700	0.85564100	0.63329500
H	2.26936700	1.89523300	0.59495900
C	2.60353400	0.09898100	-0.54613300
C	1.89068300	-1.25099900	-0.80786900
H	2.09173200	-1.94692000	0.01649800
H	2.30491200	-1.71305100	-1.71184000
C	2.50029700	0.20902200	1.92729300
H	2.66057700	0.97502900	2.69287500
H	1.79725900	-0.51559800	2.35084500
C	3.81851300	-0.49266700	1.51694400
H	4.67427400	-0.19070100	2.12939600
H	3.72881200	-1.58154900	1.59815400
C	4.01998000	-0.11096500	0.04206700
H	4.54991600	0.85051500	-0.01606000
C	2.69285400	0.92015900	-1.84330600
H	3.35160500	0.42133600	-2.56435000
H	1.72029900	1.04868600	-2.32535400
H	3.10373500	1.91759300	-1.64631100
O	4.76896800	-1.08035400	-0.71655500
H	5.68367300	-1.06406100	-0.40005700
O	-5.96868800	-0.30865100	-0.15208300
H	-6.34798700	-1.19733000	-0.07322200

Table S2. Salient physical parameters of TNTs, AC, and TNTs@AC.

Material	BET surface area (m ² /g)	Single point total pore volume (cm ³ /g)	Average pore diameter (nm)	Point of zero charge (pH _{PZC})
TNTs@AC ^[1]	471.6	0.52	3.74	3.1
TNTs ^[1]	272.3	1.26	18.6	2.6
AC ^[2]	536.1	0.60	-	6.8

Table S3. Parameters of pseudo-first-order and pseudo-second-order kinetic models for E2 adsorption onto TNTs@AC.

Kinetic models	Parameters	Initial E2 concentration (mg/L)	
		0.5	1.0
Pseudo-first-order model	$q_{e,exp}$ (mg/g)	0.999	1.908
	$q_{e,cal}$ (mg/g)	0.11	1.59
	k_1 (min ⁻¹)	0.025	0.038
	R^2	0.709	0.917
Pseudo-second-order model	$q_{e,cal}$ (mg/g)	1.01	2.01
	k_2 (g/(mg·min))	0.208	0.021
	R^2	0.999	0.998

$q_{e,cal}$ refers to the equilibrium adsorption calculated from kinetic models. $q_{e,exp}$ refers to the experimental equilibrium adsorption.

Reference

1. Liu, W.; Cai, Z.; Zhao, X.; Wang, T.; Li, F.; Zhao, D. High-Capacity and Photoregenerable Composite Material for Efficient Adsorption and Degradation of Phenanthrene in Water. *Environ. Sci. Technol.* **2016**, *50*, 11174–11183, doi:10.1021/acs.est.6b02623.
2. Ji, H.; Xie, W.; Liu, W.; Liu, X.; Zhao, D. Sorption of dispersed petroleum hydrocarbons by activated charcoals: Effects of oil dispersants. *Environ. Pollut.* **2020**, *256*, 113416, doi:https://doi.org/10.1016/j.envpol.2019.113416.