Supporting Information

Multiradical-Stabilized Hollow Carbon Sphere as Pressure-Resistant Cathode for Fast Lithium/Sodium Storage with Excellent Performance

*Chengyi Lu, [*ab] Guang Pan ,[*ab] Zhaoyong Mao ,[ab] Liangwei Shi ,[c] Qiaogao Huang ,[ab] Wenlong Tian ,[ab] Yuli Hu ,[ab] Haitao Wu ,[d] Zhenhua Wang ,[*d] and Kening Sun [d]*

[a] *School of Marine Science and Technology, Northwestern Polytechnical University, Xi'an 710072, China.*

[b] *Key Laboratory for Unmanned underwater vehicle, Northwestern Polytechnical University, Xi'an 710072, China.*

[c] *CAS Key Laboratory of Energy Regulation Materials, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, People's Republic of China.*

[d] *School of Chemistry and Chemical Engineering, Beijing Key Laboratory for Chemical Power Source and Green Catalysis, BIT-QUB Joint Center on Novel Energy and Materials Research, Beijing Institute of Technology, Beijing, 100081, China.*

1. Experimental Section

1.1 *Preparation of Hollow Carbon Spheres (HCSs)*

Step 1

In a typical synthesis procedure, monodisperse silica spheres with a particle size of about 200 nm were synthesized by a modified Stöber method. First, tetraethoxysilane (TEOS) was distilled under vacuum, and 9 mL of TEOS was mixed with 100 mL of absolute ethanol (abs. EtOH) and stirred at room temperature for 50 min to prepare solution A. Solution B was prepared by mixing 6.8 mL of an aqueous ammonia solution (NH_4OH, 25 wt%), 22 mL of abs. EtOH, and 38 mL of deionized water (DI water). Solution B was stirred at room temperature for 50 min at normal speed and 4 h at high speed. Then, solution A was rapidly added to solution B. The precursors were collected by centrifugation (three times with DI water and twice with abs. EtOH) and finally dried under vacuum at 50 ℃ for 24 h.

Step 2

First, 170 mg of 2-amino-2-hydroxymethylpropane-1,3-diol (Tris), 260 mg of triblock copolymer PEO-PPO-PEO (P123), and 500 mg of 200-nm monodisperse silicon dioxide spheres were dissolved in 170 mL of DI water and stirred vigorously at room temperature for 10 h. Then, 300 mg of dopamine hydrochloride was dispersed in the mixed solution, which was stirred at room temperature for 40 h. The particles were separated by centrifugation, washed three times with DI water and twice with abs. EtOH, and then dried under vacuum at 50 ℃ for 24 h. After that, the dried particles were heated in Ar atmosphere at 400 ℃ (reached by applying a heating rate of 1 ℃ min^{-1}) for 3 h and then further calcined at 800 ℃ (reached by applying a heating rate of 5 ℃ min^{-1}) for 5 h. Finally, the resulting powder was immersed in 8% HF solution and etched at 20 ℃ for 10–12 h. After collection by centrifugation (three times washing with DI water and twice washing with abs. EtOH) and vacuum drying at 24 ℃ for 24 h, the HCSs were obtained as final product.[2-5]

1.2 *Preparation of carboxylated Hollow Carbon Sphere (COOH–HCSs)*

In a typical synthesis procedure, 1.1 g of HCSs is first added to 76.0 mL of condensed H_2SO_4 (98 wt%), and then 3.2 g of $KMnO_4$ is added. A sealing film was used to prevent H_2SO_4 from contact with moisture in the air, and the suspension was mechanically stirred for six days to ensure complete reaction with H_2SO_4. Then, 8.0 mL of DI water was added ten times every 5 min, and the temperature was increased to about 70 ℃. Finally, since the concentration of H_2SO_4 was less than 70 wt% after a short time, 150.0 mL of DI water was added to stop the

oxidation and avoid H_2SO_4 to lose its oxidizing ability. The suspension was continuously stirred for 48 h until the temperature was below 30 ℃. After adding 13.0 mL of H_2O_2 (30 wt%), performing low-speed centrifugation, and washing with DI water, clean COOH–HCSs were obtained.[6]

1.3 *Preparation of NO-radical Hollow Carbon Sphere (TEMPO–HCSs)*

To prepare TEMPO–HCSs, 170 mL of the COOH-HCSs dispersion was added to a dry round-bottom flask. Then, 80 mL of thionyl chloride ($SOCl_2$) and 2 mL of anhydrous dimethylformamide (DMF) were added, and the mixture was stirred under reflux at 70 ℃ for 48 h. After the reaction was completed, the reaction mixture was filtered through a 0.22-μm organic-phase filter, washed with anhydrous tetrahydrofuran (THF), and dried in a vacuum oven at 25 ℃ to obtain COCl-HCS. Then, 50 mL of THF, 1.27 g of 4-hydroxy-2,2,6,6-tetramethylpiperidine-1-oxy (HTEMPO), 113.3 mg of dimethylaminopyridine (DMAP), and 1.2 mL of triethylamine (Et_3N) were added, and the resulting reaction mixture was kept under nitrogen while ensuring that the reaction temperature is lower than 5 ℃. After adding COCl-HCS, the mixture was stirred at 0 ℃ for 8 h, heated to 70 ℃, and refluxed for 60 h, and a gradual change of the colour of the reaction solution from brown to black was observed. Finally, the resulting suspension was filtered through a 0.22-μm filter membrane and washed 3–5 times with THF and five times with DI water. After drying under vacuum at 25 ℃ for 12 h, the product TEMPO–HCSs was obtained.[7]

1.4 *Materials characterization*

The prepared TEMPO–HCSs powders were also observed using scanning electron microscopy (SEM, QUANTA FEG 250 equipped with an energy dispersive spectrometer). The crystal structure of TEMPO–HCSs was characterized by powder X-ray diffraction (X'Pert PRO MPD), and the XRD data were collected at a scan rate of 1° min^{-1} in the 2θ range of 10-80°. TEM and high-resolution transmission electron microscopy (FEI TECNAI G2 T20). TGA thermal analyses were performed with TG/DTA6200 instrument at a rate of 10℃/min under nitrogen. Using Fourier transform infrared spectroscopy instrument (FTIR, IRAffinity-1, SHIMADZU) detect the nitroxide radical on TEMPO–HCSs. Electron spin resonance (ESR) spectra were obtained using a JEOL JES-TE200 ESR spectrometer with 100 kHz field modulation. X-ray photoelectron spectroscopy (XPS, VG ESCALAB MK II) was performed to determine the degree of carbon, oxygen, nitrogen and elemental composition of the obtained materials.

1.5 *Electrochemical measurements*

According to the positive active material TEMPO–HCSs: acetylene black: polyvinylidene fluoride (PVDF) at a weight ratio of 8:1:1 in NMP (N-methyl pyrrolidone, 99%) which was used as solvent to make a slurry. Then the slurry was pasted onto the aluminium foil and dried under vacuum for about 12 hours at 100℃.

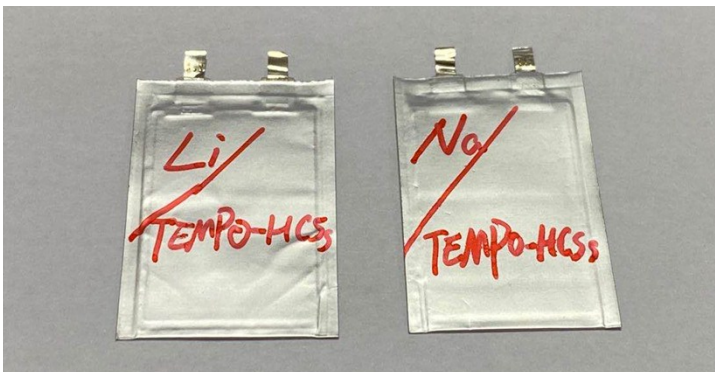
Li/ TEMPO–HCSs

The lithium metal was used as anode, and the electrolyte consists of 1mol/L, $LiPF_6$ and EC (ethylene carbonate) +DEC (Diethyl carbonate) +DMC (dimethyl carbonate) (volume ratio 1:1:1). The membrane is Celgard 2400 microporous polypropylene film. A pouch battery cells were assembled in an argon-filled glovebox with oxygen and water content below 0.5 p.p.m. The TEMPO–HCSs discharge/charge tests were conducted at various rates within a voltage window from 2.0 to 4.0 V (vs Li^+/Li) on the BTS battery testing system (Landian, Wuhan, China). The Cyclic voltammetry (CV) measurements were performed using the same cell configuration with potential galvanostatic tests in the voltage range from 2.0 V to 4.0 V at a different scan rate of 0.5 mV s^{-1} to 100 mV s^{-1}.

Na/ TEMPO–HCSs

The sodium metal was used as anode, and the electrolyte consists of 1mol/L, $NaClO_4$ and EC (ethylene carbonate) +DEC (Diethyl carbonate) (volume ratio 1:1:1, add 2% Fluoroethylene carbonate). The membrane is Celgard 2400 microporous polypropylene film. A pouch battery cells were assembled in an argon-filled glovebox with oxygen and water content below 0.5 p.p.m. The TEMPO–HCSs discharge/charge tests were conducted at various rates within a voltage window from 2.0 to 4.0 V (vs Na^+/Na) on the BTS battery testing system (Landian, Wuhan, China). The Cyclic voltammetry (CV) measurements were performed using the same cell configuration with potential galvanostatic tests in the voltage range from 2.0 V to 4.0 V at a different scan rate of 0.5 mV s^{-1} to 100 mV s^{-1}.

The weight of active material has been controlled on each electrode between 1.87 to 2.53 mg/cm^2.



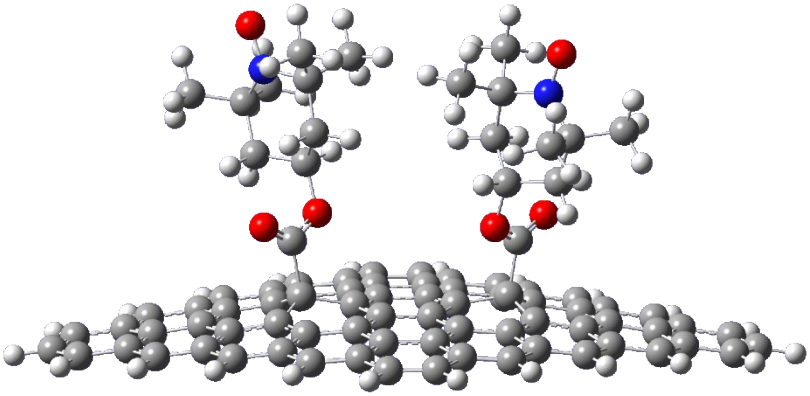
Supplementary scheme 1. The pouch battery cells of Li/TEMPO–HCSs and Na/TEMPO–HCSs.

2. Optimized geometries, cartesian coordinates (Å)

Optimized structures, geometries, cartesian coordinates (Å), and calculated thermochemical results at B3LYP/6-31G(d) level of theory with Gaussian 03

(1) Model1

Model1 with two target molecules arranged in opposite direction



E(UB3LYP) = -4024.33654573a.u.

C	-9.77471100	-2.46488000	1.48832000
C	-8.93680000	-2.30616800	2.58883300
C	-7.53876500	-2.09724400	2.42293600
C	-6.99862600	-2.02842700	1.08212400
C	-7.87858200	-2.23467000	-0.04828000
C	-9.26663900	-2.43861900	0.19234300
C	-7.33817200	-2.25716200	-1.33588500
C	-5.95316400	-2.07230700	-1.57014200
C	-5.08734700	-1.78915500	-0.45200000
C	-5.63226000	-1.79009500	0.88181700
C	-3.72221700	-1.56132300	-0.67207700
C	-3.15983500	-1.71987500	-1.95116800
C	-4.01806600	-2.01032500	-3.06889900
C	-5.39613000	-2.14731900	-2.85568700
C	-3.43730500	-2.14628600	-4.36020900
C	-2.07505100	-2.06695600	-4.55776800
C	-1.19919800	-1.82711300	-3.43044100
C	-1.74104000	-1.63109900	-2.15343900
C	-4.74697700	-1.65229800	2.00949300
C	-5.27876500	-1.78490300	3.34247000
C	-6.67167200	-1.98099500	3.51127100

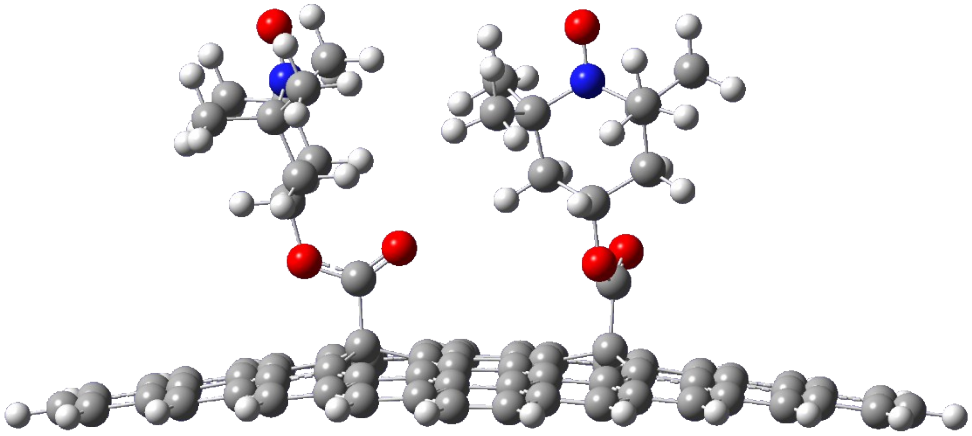
C	-3.38036000	-1.41148000	1.82662200
C	-2.87397200	-1.00116700	0.45938000
C	-1.39180300	-1.26488100	0.27069800
C	-0.86575800	-1.43957000	-1.01876800
C	0.54891300	-1.45177400	-1.20875300
C	1.09133300	-1.66258300	-2.53261500
C	0.22750000	-1.84601200	-3.62127500
C	-4.40215300	-1.69573900	4.43368200
C	-3.02395000	-1.52600100	4.25475700
C	-2.50015300	-1.39189600	2.92107200
C	-1.08204700	-1.27802600	2.72840000
C	-0.53978400	-1.26219200	1.38770900
C	0.87458400	-1.27660800	1.19774800
C	1.40074500	-1.29140100	-0.10347400
C	2.51005000	-1.79727000	-2.70722300
C	3.39039400	-1.65339200	-1.62203500
C	2.88195900	-1.05468900	-0.32754700
C	-0.21801500	-1.29567400	3.83203700
C	-0.75958500	-1.36646100	5.17164900
C	-2.12225500	-1.47543800	5.35276600
C	1.20867000	-1.30248400	3.64021500
C	1.75010900	-1.29773700	2.34815300
C	3.16892400	-1.41516800	2.16112200
C	3.73120700	-1.44587000	0.87268100
C	5.09697800	-1.69960300	0.68760700
C	5.64298600	-1.88530600	-0.63258400
C	4.75809200	-1.91157100	-1.76882300
C	0.76937400	-2.11242800	-4.93584000
C	-0.14556000	-2.27701500	-6.04369400
C	-1.48712400	-2.25423100	-5.86582100
C	3.03474800	-2.12164000	-4.00748200
C	2.13271700	-2.23952900	-5.09991800
C	5.29121500	-2.23025100	-3.06922900
C	4.41422300	-2.30609500	-4.16107900
C	7.01088600	-2.14038300	-0.79731800

C	7.55290500	-2.39131000	-2.11545100
C	6.68588800	-2.43733900	-3.20902700
C	8.95295200	-2.60878800	-2.25047300
C	9.79070000	-2.60573400	-1.13837800
C	9.28068500	-2.40540100	0.14149700
C	7.89070300	-2.18124100	0.35118300
C	7.34889100	-2.02814000	1.62928500
C	5.96284800	-1.81804100	1.83482700
C	5.40538100	-1.70830200	3.11787900
C	4.02748500	-1.53996000	3.30917800
C	3.44700400	-1.48193500	4.60660200
C	2.08493600	-1.37183700	4.79038500
C	0.15560900	-1.35979000	6.29146800
C	1.49713000	-1.36100100	6.11190800
H	-10.83861700	-2.62295000	1.64344000
H	-9.92728700	-2.58376800	-0.65826000
H	-7.99331800	-2.43883200	-2.18484300
H	-6.04740700	-2.34187200	-3.70492500
H	-4.09122500	-2.34276500	-5.20710200
H	-2.15829600	-2.40008000	-6.70862100
H	0.27735400	-2.44129100	-7.03172300
H	2.53579900	-2.45719900	-6.08658900
H	4.81388800	-2.52639500	-5.14837900
H	7.08778500	-2.64557200	-4.19795100
H	9.35984200	-2.78587400	-3.24247300
H	10.85619700	-2.77407000	-1.27005500
H	9.94142000	-2.42553900	1.00408300
H	8.00419700	-2.08478700	2.49545800
H	6.05668300	-1.77726700	3.98634600
H	4.10098100	-1.55115500	5.47317700
H	2.16850300	-1.37697800	6.96693200
H	-0.26694200	-1.37470700	7.29310300
H	-2.52485800	-1.54641700	6.36085300
H	-4.80118500	-1.77276900	5.44257600
H	-7.07222200	-2.04975000	4.52008400

H	-9.34176100	-2.34699300	3.59645500
O	-4.52938800	6.16059800	-1.88889700
N	-4.13523000	4.99097200	-1.53217900
C	-2.76905000	4.93008200	-0.90789900
C	-2.52292900	3.53468300	-0.29116800
H	-1.45710500	3.44132900	-0.05103700
H	-3.08034800	3.44316600	0.64404300
C	-2.95216500	2.41129400	-1.22840900
H	-2.38154700	2.46049700	-2.15922100
C	-4.44544100	2.51289000	-1.52252400
H	-4.75835700	1.68252600	-2.16573300
H	-4.99409400	2.42745000	-0.58031700
C	-4.81863000	3.84058200	-2.21551900
C	-2.73964000	5.98504700	0.21057800
H	-2.89756200	6.98419100	-0.19924500
H	-3.52396100	5.78592900	0.94790200
H	-1.77068300	5.95592800	0.72105100
C	-1.71330900	5.28929200	-1.97550900
H	-0.73228700	5.41928100	-1.50454600
H	-1.61402900	4.52035000	-2.74803700
H	-1.99289200	6.22873000	-2.46015400
C	-4.43598900	3.83766700	-3.71144600
H	-3.38786600	3.57048300	-3.87832800
H	-5.05544500	3.11501700	-4.25417100
H	-4.60851900	4.83209600	-4.13212600
C	-6.33304300	4.07078100	-2.08113700
H	-6.62125600	4.13574700	-1.02690000
H	-6.87443300	3.23489600	-2.53742400
H	-6.62475100	4.99885200	-2.57604300
C	-3.12880700	0.57377500	0.36700500
O	-3.77971300	1.19263100	1.17594000
O	-2.58550400	1.07982300	-0.75028700
O	4.52002600	6.34836400	1.07700800
N	4.12357700	5.14479000	0.86529700
C	2.79977500	5.01280300	0.16392200

C	2.56316000	3.54669700	-0.26339900
H	1.51367500	3.43366400	-0.56055200
H	3.17843000	3.31379800	-1.13575800
C	2.90275000	2.56440300	0.85227100
H	2.27073800	2.75340100	1.72372800
C	4.37410100	2.68862800	1.23463300
H	4.62361000	1.95479900	2.00951600
H	4.98505900	2.46287000	0.35585700
C	4.72778400	4.09693800	1.75710800
C	2.86608600	5.89707500	-1.09250500
H	3.01957400	6.94254200	-0.81923100
H	3.69132200	5.58436800	-1.74032100
H	1.93090000	5.80737100	-1.65624400
C	1.68501500	5.53430600	1.09574200
H	0.74062700	5.60970700	0.54511200
H	1.51842700	4.88341100	1.95943900
H	1.95404700	6.52907100	1.46137300
C	4.23815800	4.31602700	3.20490100
H	3.17466400	4.09042100	3.32986600
H	4.79886900	3.67142400	3.89096300
H	4.40455900	5.35857400	3.48996900
C	6.25306800	4.28486000	1.70573200
H	6.61830500	4.19380400	0.67770300
H	6.73875300	3.51547700	2.31578100
H	6.53082000	5.26999400	2.08465500
C	3.14616500	0.51659200	-0.45057900
O	3.85813500	1.00721600	-1.29525300
O	2.54058500	1.18194500	0.54403100

Model1 with two target molecules arranged in crossing mode



E(UB3LYP) = -4024.34037278a.u.

C	-9.24213800	-2.99712400	1.79390700
C	-8.54731300	-2.26113200	2.74999600
C	-7.16883400	-1.95026600	2.57832700
C	-6.49895100	-2.39567400	1.37481400
C	-7.22829700	-3.19045500	0.40946200
C	-8.60506400	-3.46311000	0.64688000
C	-6.55686000	-3.68358400	-0.71101800
C	-5.18288900	-3.41985800	-0.93827500
C	-4.47197200	-2.57253000	-0.01384100
C	-5.15242100	-2.07812100	1.15593800
C	-3.12673700	-2.26185700	-0.25111400
C	-2.42561600	-2.86324900	-1.31220700
C	-3.12993300	-3.71082200	-2.23828100
C	-4.49711000	-3.94410200	-2.04473700
C	-2.41053000	-4.28707300	-3.32161100
C	-1.05036300	-4.11173200	-3.46949000
C	-0.32135100	-3.31720300	-2.50454700
C	-1.00796500	-2.68599200	-1.45792100
C	-4.41348900	-1.33651500	2.14586500
C	-5.06467300	-0.95547400	3.37450000
C	-6.44026800	-1.25192200	3.54322700
C	-3.06572200	-1.01068000	1.94571900
C	-2.44404000	-1.17981700	0.56787700
C	-0.93922400	-1.33971000	0.61723100

C	-0.27344300	-1.95015200	-0.45502200
C	1.14643500	-1.85271400	-0.55177600
C	1.83891800	-2.50315600	-1.64043900
C	1.11246200	-3.22632700	-2.59536300
C	-4.31899800	-0.29135900	4.36062700
C	-2.94933000	-0.04490500	4.20382200
C	-2.30469600	-0.42573100	2.97450700
C	-0.88572700	-0.25149300	2.83913700
C	-0.21254800	-0.75348700	1.66338100
C	1.20682100	-0.65510700	1.56876600
C	1.85868000	-1.14236500	0.42628300
C	3.27397900	-2.48918600	-1.68115200
C	4.01793300	-1.77696100	-0.72615500
C	3.31374400	-0.78629000	0.17543400
C	-0.14047700	0.30536600	3.88718900
C	-0.80847400	0.74692200	5.09231700
C	-2.16994400	0.56881200	5.22330200
C	1.29335900	0.39828800	3.79297300
C	1.95985500	-0.06566700	2.65191000
C	3.39379600	-0.03764900	2.58944900
C	4.07933200	-0.49958800	1.45160300
C	5.47684100	-0.59371900	1.44547000
C	6.17114600	-1.21897200	0.34828200
C	5.41488800	-1.85193500	-0.70188200
C	1.80963200	-3.92839300	-3.65118100
C	1.03176500	-4.65323800	-4.63156500
C	-0.31655500	-4.73925100	-4.54666700
C	3.95897600	-3.23409600	-2.70318800
C	3.18826000	-3.91894800	-3.68347200
C	6.10907200	-2.59394800	-1.72486900
C	5.35930300	-3.25118400	-2.71220800
C	7.57012500	-1.30518000	0.35854400
C	8.26671500	-1.99190800	-0.70778200
C	7.52529400	-2.62029300	-1.71114900
C	9.68951400	-2.02690100	-0.68449700

C	10.40534500	-1.43602800	0.35315300
C	9.74968900	-0.80661900	1.40805500
C	8.32892600	-0.73326800	1.45007500
C	7.64697800	-0.15550100	2.52381300
C	6.23213400	-0.09777400	2.56982700
C	5.54088000	0.43545500	3.66829200
C	4.14070600	0.45201700	3.71687800
C	3.42937600	0.95205900	4.84342100
C	2.05158900	0.93648200	4.90157400
C	-0.01387500	1.33163600	6.15028700
C	1.33406800	1.42030300	6.06049700
H	-10.29404200	-3.22066100	1.95052800
H	-9.15329600	-4.05236100	-0.08339200
H	-7.09740500	-4.29816000	-1.42731000
H	-5.03594600	-4.56562900	-2.75643400
H	-2.95184200	-4.90423700	-4.03542700
H	-0.88088400	-5.30548300	-5.28350400
H	1.56608700	-5.14860400	-5.43851900
H	3.70945300	-4.45930100	-4.47071300
H	5.87897100	-3.79375000	-3.49872500
H	8.04711700	-3.15397200	-2.50221200
H	10.21188800	-2.53305800	-1.49192400
H	11.49127800	-1.47750900	0.34616700
H	10.31882500	-0.36768700	2.22323100
H	8.21499000	0.24979500	3.35813500
H	6.10607700	0.82936300	4.51004400
H	3.99669100	1.34405300	5.68484600
H	1.91357200	1.84742300	6.87530100
H	-0.53184600	1.68560200	7.03826900
H	-2.66548100	0.88083000	6.14011600
H	-4.81200600	0.01682700	5.27995100
H	-6.93538700	-0.93618300	4.45871300
H	-9.05070600	-1.91874200	3.65023200
O	-5.28070800	5.17857000	-2.88702800
N	-4.87237400	4.10141200	-2.31836300

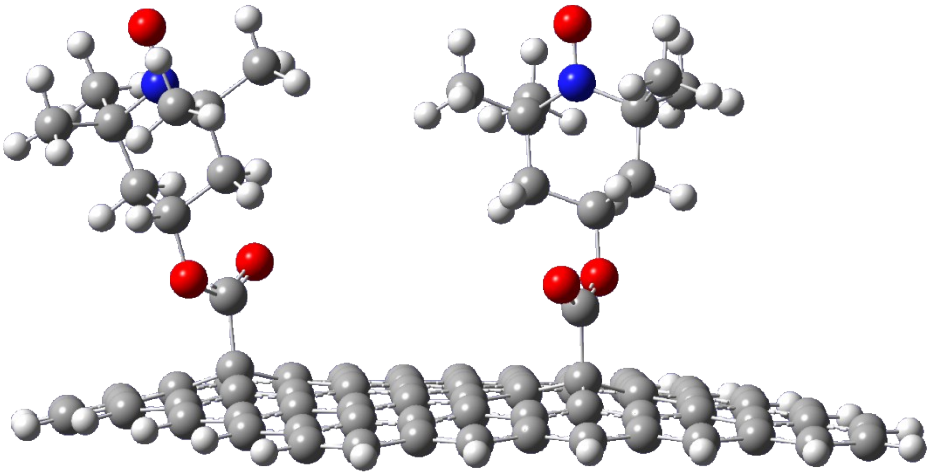
C	-4.80404700	2.88779600	-3.20404600
C	-4.06663500	1.74083900	-2.47870800
H	-4.22725200	0.81231200	-3.03856200
H	-2.99107900	1.93879700	-2.47126800
C	-4.54631500	1.57611200	-1.04132600
H	-5.61633300	1.35439800	-1.02877900
C	-4.26928000	2.84433800	-0.24218900
H	-4.57687100	2.70835500	0.80106500
H	-3.19263800	3.03432100	-0.24616400
C	-5.01558800	4.06628700	-0.82161700
C	-4.00917200	3.28718900	-4.45802000
H	-4.51887400	4.08862500	-4.99574700
H	-3.00813800	3.63742100	-4.18664700
H	-3.90606400	2.42007900	-5.11938300
C	-6.23463200	2.48220900	-3.61980900
H	-6.19365800	1.70985000	-4.39588400
H	-6.82177700	2.08701800	-2.78503500
H	-6.75525200	3.35535100	-4.02253100
C	-6.51547000	4.05237400	-0.45588000
H	-7.00722100	3.11334600	-0.72759300
H	-6.63862500	4.19551800	0.62337700
H	-7.02272700	4.86869200	-0.97736200
C	-4.37614700	5.35408400	-0.27667900
H	-3.32379900	5.41869900	-0.57178400
H	-4.43114300	5.35782400	0.81745500
H	-4.89552200	6.23256900	-0.66369800
C	-2.70434300	0.20989200	-0.18008500
O	-1.83097500	0.99485400	-0.47450200
O	-4.01281200	0.37646500	-0.40446200
O	1.90563300	6.30287800	-2.64431100
N	2.16177600	5.16041600	-2.11496100
C	0.96317100	4.32100700	-1.76893000
C	1.40188100	2.89364300	-1.37752600
H	0.55116300	2.37474600	-0.92162500
H	1.68301600	2.33903700	-2.27726300

C	2.59044900	2.91310200	-0.42405000
H	2.33165900	3.45838100	0.48700900
C	3.79508000	3.56112500	-1.09686000
H	4.66407000	3.53219700	-0.42915000
H	4.04730900	2.98697400	-1.99231300
C	3.51859900	5.03144400	-1.48051200
C	0.08406100	4.24909400	-3.02808300
H	-0.26062900	5.24450000	-3.31451300
H	0.64477700	3.82182700	-3.86568900
H	-0.78299500	3.60985800	-2.82961200
C	0.17305200	5.01174500	-0.63693000
H	-0.77530900	4.48804000	-0.47289600
H	0.71691500	5.02018400	0.31294300
H	-0.03800700	6.04670400	-0.92036100
C	3.59426000	5.96974400	-0.25662900
H	2.95157500	5.64056600	0.56597200
H	4.62286400	6.01415700	0.11854600
H	3.28486200	6.97600600	-0.55204200
C	4.55085200	5.48163100	-2.52762300
H	4.47829900	4.86512600	-3.42944800
H	5.56137000	5.37832900	-2.11729000
H	4.38309400	6.52320000	-2.80777200
C	3.22778700	0.56976100	-0.66806300
O	3.40345800	0.62365200	-1.86268900
O	2.89057100	1.59293900	0.12475900

==========

(2) Model2

Model2 with two target molecules arranged in opposite direction



E(UB3LYP) = -4024.31772556a.u.

O	-2.00974300	6.72330200	-1.74898300
N	-2.31064800	5.52804600	-1.38618800
C	-3.75312700	5.30436500	-1.02575600
C	-4.03389700	3.79534300	-0.85779800
H	-5.01063600	3.67303300	-0.37558700
H	-4.08852000	3.32055100	-1.84078300
C	-2.95263700	3.09989200	-0.03813100
H	-2.89794900	3.53971200	0.96076500
C	-1.60264500	3.21945300	-0.73602400
H	-0.83471800	2.68491600	-0.16503800
H	-1.67288500	2.74766000	-1.71999200
C	-1.16174200	4.69104600	-0.89592200
C	-4.59856200	5.84599700	-2.19039000
H	-4.42538400	6.91518000	-2.32539100
H	-4.34220500	5.33377400	-3.12338300
H	-5.66104400	5.67769500	-1.98327100
C	-4.08432000	6.10068200	0.25502600
H	-5.16473300	6.08433600	0.43689800
H	-3.58905300	5.69632000	1.14341600
H	-3.76639300	7.13922500	0.12819500
C	-0.63237500	5.28247900	0.42815400
H	-1.33866200	5.16399500	1.25579900
H	0.30225100	4.78634300	0.71202100

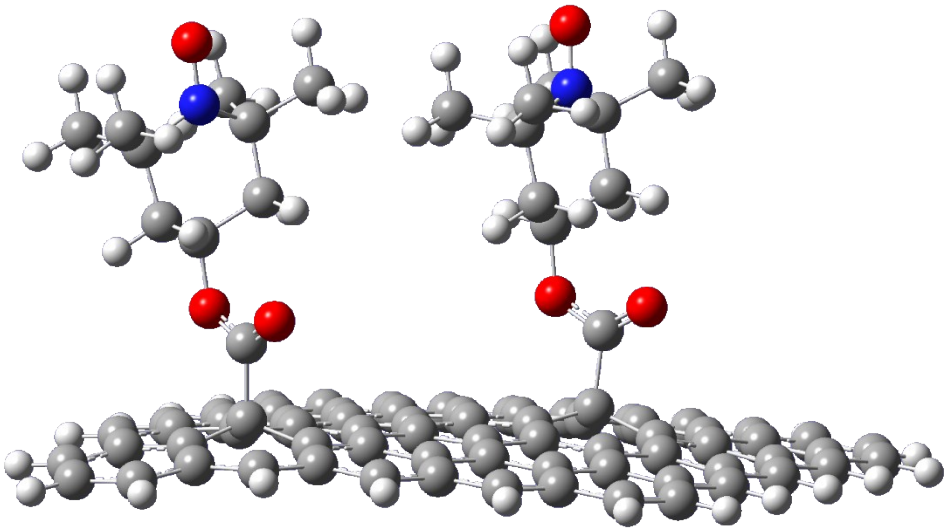
H	-0.43613500	6.34985000	0.29465200
C	-0.05701500	4.77276500	-1.96255700
H	-0.42519200	4.41028900	-2.92777300
H	0.79297500	4.15158300	-1.65873000
H	0.28005800	5.80342900	-2.08675700
C	-3.45260300	0.79622700	-0.66978200
O	-3.38401200	0.99423400	-1.86034700
O	-3.29284600	1.71704100	0.28969800
C	-10.77885900	-0.90130800	-0.50625900
C	-10.18594400	-0.47341100	0.67905600
C	-8.77406900	-0.49520400	0.84147200
C	-7.95348900	-0.94734600	-0.25971300
C	-8.58787000	-1.42989900	-1.46580600
C	-10.00547300	-1.38005500	-1.56049200
C	-7.79219400	-1.95709800	-2.48961200
C	-6.38352100	-2.01685900	-2.38712000
C	-5.74282700	-1.46571000	-1.21757500
C	-6.55418400	-0.94486400	-0.14795200
C	-4.34660000	-1.46965000	-1.12404400
C	-3.55757900	-2.09132900	-2.10865300
C	-4.19091500	-2.65449000	-3.27345900
C	-5.58363400	-2.58212600	-3.39435800
C	-3.37832400	-3.25533300	-4.27465000
C	-2.00767600	-3.35364500	-4.14165100
C	-1.36655000	-2.83734300	-2.95121400
C	-2.13688200	-2.19532900	-1.96005600
C	-5.92780500	-0.52865600	1.08059600
C	-6.75373300	-0.15948300	2.20532800
C	-8.15770700	-0.12379400	2.04228600
C	-4.53343700	-0.51574300	1.20849600
C	-3.67804700	-0.65648500	-0.03459800
C	-2.26471800	-1.11898500	0.26872200
C	-1.50509200	-1.73042400	-0.74957800
C	-0.11247900	-1.93625000	-0.56074300
C	0.66839900	-2.55382900	-1.58667200

C	0.03883600	-3.00664800	-2.77824600
C	-6.13395700	0.16433200	3.42376500
C	-4.74424900	0.09564900	3.58311800
C	-3.92528900	-0.26210600	2.45357400
C	-2.50730900	-0.37064800	2.61865300
C	-1.68932500	-0.82812600	1.52204200
C	-0.29748700	-1.03005100	1.72123600
C	0.50944900	-1.53180700	0.65738200
C	2.06454600	-2.72629400	-1.40731300
C	2.70679300	-2.24183900	-0.22350900
C	1.91038800	-1.66780400	0.82517900
C	-1.91811300	-0.11401800	3.87380800
C	-2.74516000	0.29536900	4.98866700
C	-4.11320700	0.38639500	4.82464700
C	-0.51354200	-0.27576700	4.06014000
C	0.29872700	-0.73134400	2.98594900
C	1.69490300	-0.89885300	3.16836700
C	2.51938500	-1.33041500	2.08145800
C	3.90389900	-1.44637600	2.25950200
C	4.79632500	-1.65679900	1.05649400
C	4.09567300	-2.37155300	-0.07873000
C	0.82321600	-3.65517400	-3.79109900
C	0.15502600	-4.12292900	-4.98408700
C	-1.18394600	-3.98272800	-5.14717400
C	2.84108900	-3.37657200	-2.42087600
C	2.18699200	-3.82711000	-3.59679800
C	4.86262800	-3.08524500	-1.04700100
C	4.21910400	-3.56602400	-2.20397200
C	6.13754700	-2.27716200	1.41220200
C	6.86292400	-2.99805700	0.43014800
C	6.24133700	-3.33118200	-0.80475800
C	8.18672500	-3.41296100	0.73383700
C	8.75206000	-3.13558900	1.97590000
C	8.01794800	-2.47224200	2.95526200
C	6.68870300	-2.04299700	2.69751900

C	5.88859800	-1.44359300	3.70944300
C	4.49665800	-1.21348600	3.53359000
C	3.67557600	-0.79912700	4.60058900
C	2.28970800	-0.61416500	4.44053700
C	1.45507800	-0.17012200	5.49901100
C	0.08737400	0.00063900	5.33445500
C	-2.10420300	0.57701400	6.25180400
C	-0.76461600	0.44231200	6.41502100
H	-11.86079600	-0.87413300	-0.60447300
H	-10.48038600	-1.73261400	-2.47223400
H	-8.26981000	-2.34332500	-3.38719300
H	-6.06067200	-2.98307400	-4.28585400
H	-3.86038200	-3.65620900	-5.16367500
H	-1.67091100	-4.35255600	-6.04619200
H	0.75617800	-4.60463000	-5.75133400
H	2.77593300	-4.32562100	-4.36367400
H	4.80318700	-4.10117600	-2.94924900
H	6.81479200	-3.87673900	-1.55002900
H	8.75069300	-3.96120200	-0.01633100
H	9.76829100	-3.45632000	2.18885300
H	8.44937300	-2.28663700	3.93529400
H	6.33228500	-1.25140700	4.68295800
H	4.12570600	-0.61346200	5.57298400
H	1.90594700	0.03923600	6.46661200
H	-0.30224800	0.65664200	7.37543200
H	-2.73044000	0.89842400	7.08048800
H	-4.73541000	0.67970400	5.66750000
H	-6.75128100	0.46018500	4.26909300
H	-8.77557000	0.18741700	2.88159100
H	-10.80103200	-0.12374000	1.50401800
O	7.39760300	4.76488000	-2.45418500
N	6.96638200	3.66554200	-1.94803200
C	8.02508800	2.73715600	-1.42140700
C	7.37604900	1.58873200	-0.61903000
H	8.13041800	0.81270900	-0.44467600

H	7.05317100	1.96123600	0.35685500
C	6.17102400	0.99678700	-1.34144500
H	6.47547600	0.59491800	-2.31123400
C	5.09524900	2.06030300	-1.53093200
H	4.21363900	1.62291700	-2.01376500
H	4.78704100	2.42594800	-0.54804600
C	5.59299300	3.24287100	-2.39120400
C	8.92210700	3.56135400	-0.48286500
H	9.40797700	4.37187900	-1.02903700
H	8.33158900	3.99743700	0.32927600
H	9.68937500	2.91347500	-0.04499900
C	8.87156900	2.21321900	-2.60138900
H	9.74960100	1.67744100	-2.22370100
H	8.31486300	1.52911400	-3.24932600
H	9.21083300	3.05885000	-3.20594800
C	5.63281000	2.88888800	-3.89322200
H	6.20558200	1.97868600	-4.09642000
H	4.61517100	2.73602400	-4.26934500
H	6.09047400	3.71287600	-4.44751600
C	4.65984300	4.44652500	-2.17938900
H	4.65756600	4.75241100	-1.12811700
H	3.63735500	4.17483200	-2.46424300
H	4.98443200	5.29502600	-2.78428200
C	5.18434200	-0.17788700	0.55711800
O	5.08565200	0.80543400	1.25270700
O	5.66379000	-0.21059400	-0.69299300

Model2 with two target molecules arranged in parallel



E(UB3LYP) = -4024.30672668a.u.

O	1.94687100	-5.85746500	-3.75554200
N	2.22494600	-4.83249900	-3.03254800
C	3.49953700	-4.92482900	-2.24036400
C	3.84337200	-3.55328600	-1.61995600
H	4.63123800	-3.69572200	-0.87124900
H	4.23791200	-2.88833900	-2.39284600
C	2.62541300	-2.89414800	-0.98230300
H	2.22611900	-3.53211400	-0.18980900
C	1.55472300	-2.63800800	-2.03737500
H	0.69660700	-2.12457900	-1.58824900
H	1.96870000	-1.97905500	-2.80514400
C	1.05948500	-3.94726900	-2.68981700
C	4.61299100	-5.32615000	-3.22222000
H	4.39964100	-6.29971600	-3.66724900
H	4.70093800	-4.58983700	-4.02764900
H	5.57066200	-5.37605600	-2.69256800
C	3.34886500	-6.02362600	-1.16628800
H	4.31642500	-6.21543800	-0.68927100
H	2.63632000	-5.75110500	-0.38131200
H	3.00225900	-6.94680200	-1.63887200
C	0.09292900	-4.72134400	-1.76750300
H	0.50874100	-4.89272100	-0.76964400
H	-0.84089300	-4.15977400	-1.64877700

H	-0.13599400	-5.69185000	-2.21614800
C	0.34266300	-3.61350300	-4.00859500
H	1.02591700	-3.11413800	-4.70303900
H	-0.50007200	-2.94195300	-3.81039600
H	-0.02859300	-4.52294000	-4.48453400
C	3.48791100	-0.61574500	-0.82387800
O	3.75289200	-0.51882500	-1.99896500
O	2.96657500	-1.69423000	-0.22325800
C	10.79162100	0.42980200	0.43957800
C	10.06418200	-0.28951600	1.38420700
C	8.64441400	-0.21265300	1.43032500
C	7.96018800	0.60854300	0.45623800
C	8.73375500	1.38288400	-0.48864100
C	10.15077800	1.25908900	-0.47727200
C	8.07020400	2.24783900	-1.36496400
C	6.66111300	2.37614200	-1.36722000
C	5.88295900	1.55102900	-0.47641700
C	6.55863800	0.67584400	0.44637100
C	4.48599900	1.62813200	-0.50203200
C	3.82901000	2.56418900	-1.32006300
C	4.59939200	3.39798400	-2.20557100
C	5.99306200	3.26774300	-2.22247500
C	3.91723200	4.31825600	-3.05069200
C	2.54598700	4.46517600	-3.01570700
C	1.76566900	3.67018900	-2.09103500
C	2.40451300	2.71691500	-1.27099000
C	5.79405400	-0.04224800	1.43399400
C	6.48411900	-0.78718500	2.45874000
C	7.89562300	-0.87792300	2.40654500
C	4.39387500	0.01145800	1.43880800
C	3.67516700	0.57849300	0.22908800
C	2.26240500	1.03016000	0.53831400
C	1.63526400	1.96499800	-0.31270400
C	0.24133000	2.20524000	-0.19000400
C	-0.40366500	3.14474400	-1.04828000

C	0.35885800	3.87690500	-1.99653800
C	5.73149600	-1.40453900	3.47104800
C	4.33805400	-1.27683700	3.53325600
C	3.65401900	-0.54659100	2.49826600
C	2.23191100	-0.37908600	2.57640900
C	1.55090600	0.43283400	1.60110000
C	0.15777300	0.66646400	1.73454000
C	-0.51954200	1.50836200	0.79851900
C	-1.80559300	3.35415700	-0.94463900
C	-2.58098700	2.59864600	-0.01265300
C	-1.91667200	1.68623900	0.87959000
C	1.51173000	-0.93669200	3.65249200
C	2.20478600	-1.70929900	4.66201600
C	3.57392200	-1.85902800	4.58419000
C	0.10607000	-0.72734200	3.76611200
C	-0.57204300	0.06777000	2.80542100
C	-1.97415600	0.27683700	2.91303800
C	-2.66734300	1.04443500	1.92691600
C	-4.05654400	1.19919500	2.01164700
C	-4.81372100	1.81176300	0.85171200
C	-3.96798300	2.77776600	0.04667900
C	-0.29465500	4.84116700	-2.84026600
C	0.51172600	5.58688500	-3.78160200
C	1.85330500	5.41152300	-3.86037200
C	-2.44922700	4.31119500	-1.79052600
C	-1.66080000	5.03755700	-2.72477400
C	-4.60405600	3.76247600	-0.75233300
C	-3.83548800	4.50997000	-1.65592300
C	-6.15179500	2.40457400	1.26785100
C	-6.75403700	3.40121100	0.45397700
C	-6.00913300	4.00458600	-0.58698300
C	-8.08851400	3.80188700	0.74671900
C	-8.77738400	3.24918300	1.82262400
C	-8.16602700	2.31121400	2.64981500
C	-6.83387800	1.87655700	2.39642800

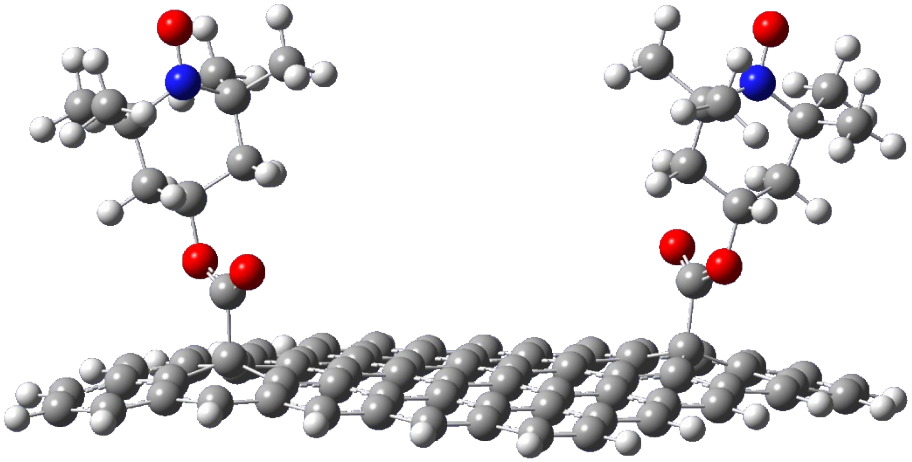
C	-6.16917000	0.97664300	3.26343400
C	-4.77044300	0.68894800	3.13012900
C	-4.08220500	-0.05228400	4.10039500
C	-2.69957400	-0.29768200	4.00377600
C	-1.99393000	-1.07921900	4.95888300
C	-0.63051200	-1.30218900	4.85952900
C	1.42990300	-2.28307600	5.73881700
C	0.09108900	-2.09382200	5.83172300
H	11.87556600	0.35321000	0.42632500
H	10.73038800	1.83225400	-1.19597400
H	8.65237800	2.84755000	-2.06087700
H	6.57500400	3.87765300	-2.90978300
H	4.50379500	4.92648400	-3.73584700
H	2.44383900	5.99115900	-4.56564500
H	0.01146000	6.30710400	-4.42428900
H	-2.15094900	5.76911200	-3.36347000
H	-4.32418500	5.25979700	-2.27386700
H	-6.48776100	4.74975200	-1.21675000
H	-8.55813900	4.55694200	0.12199400
H	-9.79613300	3.56612800	2.02929600
H	-8.69540600	1.90641000	3.50833200
H	-6.70633500	0.57099100	4.11688500
H	-4.63110600	-0.45005800	4.95112300
H	-2.54669600	-1.51087900	5.79052800
H	-0.47168900	-2.53114000	6.65279800
H	1.95580000	-2.87246600	6.48599600
H	4.09539300	-2.42735000	5.35142600
H	6.24657400	-1.97986900	4.23711900
H	8.41118300	-1.46919200	3.15992100
H	10.57663900	-0.91569200	2.10974400
O	-7.22063700	-4.50794400	-2.96165400
N	-6.80607300	-3.51137600	-2.26473600
C	-5.33679900	-3.51165300	-1.94446000
C	-4.92431700	-2.15691900	-1.32819400
H	-3.92392000	-2.26175800	-0.89225100

H	-4.86534200	-1.39871400	-2.11324900
C	-5.91175000	-1.68540800	-0.26670100
H	-5.96637900	-2.41590600	0.54467800
C	-7.29192500	-1.48477600	-0.88277100
H	-7.99034200	-1.10629700	-0.12744900
H	-7.21868600	-0.73170200	-1.67184500
C	-7.86138400	-2.79597000	-1.46751900
C	-4.58668900	-3.71062100	-3.27193800
H	-4.85453000	-4.66719800	-3.72403300
H	-4.83531600	-2.91227600	-3.97856400
H	-3.50605300	-3.69052100	-3.09196400
C	-5.02419400	-4.69381700	-1.00200400
H	-3.93982600	-4.80998600	-0.89431800
H	-5.44721100	-4.55888700	-0.00151700
H	-5.43347200	-5.61433200	-1.42712500
C	-8.38732000	-3.73925900	-0.36458000
H	-7.64266100	-3.93294100	0.41362800
H	-9.26845800	-3.29961900	0.11610300
H	-8.67255600	-4.69558600	-0.81139100
C	-9.00779400	-2.45975400	-2.43531900
H	-8.64529600	-1.83864000	-3.26073400
H	-9.78918600	-1.90693000	-1.90240600
H	-9.43686700	-3.37228000	-2.85310500
C	-5.23347900	0.65629200	-0.17776900
O	-5.38246500	0.85164400	-1.36163800
O	-5.44037600	-0.50615900	0.45656700

==========

(3) Model3

Model3 with two target molecule arranged in opposite direction



E(UB3LYP) = -4024.30898676a.u.

C	-9.86881100	-2.24286600	0.78697500
C	-9.09672100	-2.10996400	1.93784200
C	-7.70513600	-1.83750600	1.84986500
C	-7.12586600	-1.67463200	0.56556900
C	-7.89850500	-1.86012100	-0.60904200
C	-9.28567300	-2.13644200	-0.47284800
C	-7.26819400	-1.81742000	-1.88171400
C	-5.85486200	-1.73266300	-2.02228900
C	-5.04208900	-1.54878100	-0.86516900
C	-5.68940100	-1.18680800	0.45471900
C	-3.64705700	-1.60524600	-0.96054400
C	-3.02446600	-1.73785900	-2.24139800
C	-3.83607900	-1.84887100	-3.41834200
C	-5.23246400	-1.87009700	-3.27761200
C	-3.19746500	-1.95439400	-4.68531500
C	-1.81995200	-1.95070100	-4.81403400
C	-0.99625300	-1.84692600	-3.63438000
C	-1.61090900	-1.74728600	-2.35269000
C	-4.84123500	-1.56946500	1.64925100
C	-5.46195300	-1.72586200	2.92099200
C	-6.88163900	-1.78226500	3.00645400
C	-3.45011700	-1.62064500	1.52293800
C	-2.82395600	-1.57793300	0.22395900

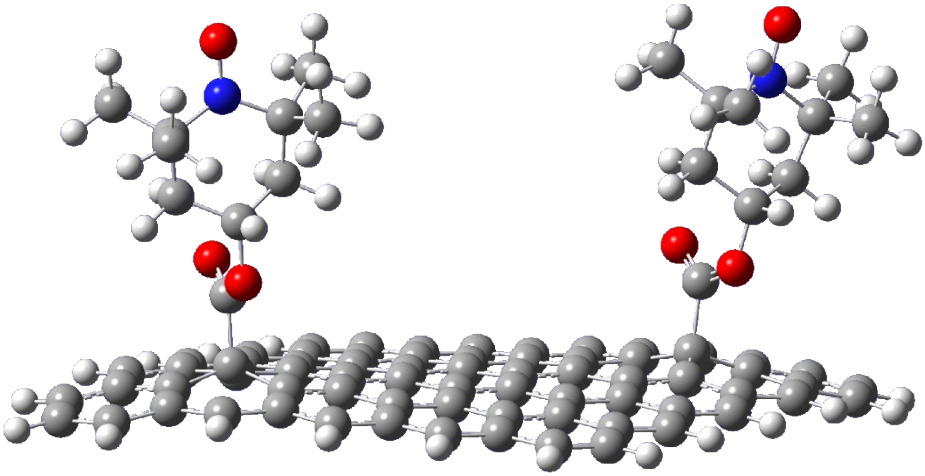
C	-1.42647600	-1.62338900	0.11321300
C	-0.80063800	-1.66844400	-1.17891600
C	0.60555700	-1.67122500	-1.29017000
C	1.22072500	-1.75413000	-2.57676200
C	0.41174900	-1.84994500	-3.74570800
C	-4.65066400	-1.86374500	4.06323600
C	-3.24991300	-1.85455500	3.98005700
C	-2.63360400	-1.74958600	2.68972100
C	-1.22042700	-1.75321800	2.57734400
C	-0.60526000	-1.67076300	1.29072200
C	0.80093400	-1.66798900	1.17946700
C	1.42677100	-1.62337700	-0.11267800
C	2.63390200	-1.75050200	-2.68914100
C	3.45041200	-1.62109400	-1.52240500
C	2.82424800	-1.57792000	-0.22343900
C	-0.41144900	-1.84857200	3.74632700
C	-1.03903400	-1.95317100	5.04090500
C	-2.41948000	-1.95832000	5.13073500
C	0.99655200	-1.84555600	3.63499700
C	1.61120700	-1.74636500	2.35327200
C	3.02476300	-1.73693900	2.24197700
C	3.64735000	-1.60476800	0.96107500
C	5.04237900	-1.54829300	0.86567900
C	5.68968100	-1.18675800	-0.45434500
C	4.84152400	-1.56991400	-1.64874100
C	1.03933800	-1.95500400	-5.04024800
C	0.18920800	-2.05559000	-6.20312000
C	-1.16364300	-2.05368400	-6.09617700
C	3.25021400	-1.85593700	-3.97943600
C	2.41978300	-1.96015000	-5.13007600
C	5.46224900	-1.72678300	-2.92041800
C	4.65096700	-1.86512500	-4.06261000
C	7.12617300	-1.67459100	-0.56501400
C	7.70544000	-1.83794800	-1.84924700
C	6.88193900	-1.78317600	-3.00585700

C	9.09702800	-2.11042200	-1.93712300
C	9.86912100	-2.24288700	-0.78620800
C	9.28598000	-2.13600700	0.47357400
C	7.89880900	-1.85965400	0.60966500
C	7.26849200	-1.81652400	1.88232200
C	5.85515900	-1.73174200	2.02286400
C	5.23276600	-1.86873900	3.27823900
C	3.83637900	-1.84749700	3.41896100
C	3.19776700	-1.95257400	4.68597200
C	1.82025400	-1.94887200	4.81469000
C	-0.18890300	-2.05330600	6.20381300
C	1.16394900	-2.05140200	6.09687000
H	-10.93221800	-2.44977500	0.87266500
H	-9.88445000	-2.27444200	-1.36935200
H	-7.87537000	-1.95288500	-2.77320100
H	-5.85203800	-1.99863500	-4.16232400
H	-3.81756800	-2.04046600	-5.57504200
H	-1.78612300	-2.13132600	-6.98426400
H	0.66405800	-2.13457000	-7.17802000
H	2.89208500	-2.04300200	-6.10654600
H	5.12368500	-1.97603200	-5.03576900
H	7.34344100	-1.89028800	-3.98410100
H	9.54863600	-2.22725400	-2.91869700
H	10.93253100	-2.44981400	-0.87182100
H	9.88475700	-2.27367100	1.37013000
H	7.87566800	-1.95164900	2.77386000
H	5.85234500	-1.99693700	4.16299500
H	3.81787400	-2.03830100	5.57573100
H	1.78643000	-2.12870000	6.98498600
H	-0.66375100	-2.13194100	7.17874300
H	-2.89178000	-2.04082500	6.10723500
H	-5.12337800	-1.97430400	5.03643600
H	-7.34314200	-1.88901600	3.98473800
H	-9.54832700	-2.22643400	2.91945900
O	-7.08852000	6.39797000	-0.39927400

N	-6.84772700	5.13681600	-0.34966000
C	-5.47519800	4.72088600	-0.80032900
C	-5.22613400	3.23665500	-0.45306100
H	-4.33123200	2.89759900	-0.98749900
H	-5.02878500	3.13877900	0.61752900
C	-6.41750100	2.35535400	-0.81210600
H	-6.61447800	2.41051900	-1.88590000
C	-7.65170900	2.79146700	-0.03027000
H	-8.49653000	2.13226200	-0.26138000
H	-7.44145400	2.69559900	1.03825600
C	-8.05879300	4.24661400	-0.34921600
C	-4.46539300	5.59145100	-0.03416800
H	-4.61544700	6.64730400	-0.26629200
H	-4.58081400	5.45512300	1.04598900
H	-3.44566200	5.30428400	-0.31285000
C	-5.33497700	4.99273600	-2.31356000
H	-4.29499400	4.84558300	-2.62546200
H	-5.96305500	4.33300100	-2.92028200
H	-5.62084200	6.02696600	-2.52415500
C	-8.77282600	4.36173000	-1.71319100
H	-8.19465000	3.91915900	-2.53041100
H	-9.74174700	3.85146300	-1.67318800
H	-8.94259700	5.41677100	-1.94519600
C	-8.99571300	4.75962800	0.75690900
H	-8.49003700	4.74328400	1.72776700
H	-9.88146600	4.11770500	0.81630700
H	-9.30953600	5.78418300	0.54923800
C	-5.84151000	0.40923700	0.54130500
O	-5.75159900	1.02494600	1.57762400
O	-6.13134600	0.93022900	-0.65842100
O	7.08733900	6.39857800	0.39730200
N	6.84680100	5.13736000	0.34789100
C	5.47430300	4.72126500	0.79853100
C	5.22563400	3.23686000	0.45172800
H	4.33069300	2.89779800	0.98609800

H	5.02852700	3.13859000	-0.61887100
C	6.41711400	2.35591300	0.81129500
H	6.61387500	2.41150900	1.88511100
C	7.65137100	2.79206900	0.02953500
H	8.49630300	2.13313300	0.26101200
H	7.44131500	2.69577700	-1.03899400
C	8.05806800	4.24741400	0.34803900
C	4.46440500	5.59131100	0.03190700
H	4.61423800	6.64728800	0.26361500
H	4.57996600	5.45455900	-1.04818100
H	3.44470000	5.30406500	0.31060400
C	5.33379200	4.99363200	2.31164600
H	4.29380500	4.84629800	2.62344600
H	5.96195700	4.33429300	2.91870700
H	5.61933600	6.02801500	2.52191400
C	8.77180000	4.36319500	1.71211800
H	8.19354800	3.92081100	2.52938400
H	9.74082400	3.85309600	1.67249900
H	8.94131800	5.41835300	1.94376700
C	8.99509000	4.76022600	-0.75809000
H	8.48962700	4.74335100	-1.72905000
H	9.88103800	4.11853200	-0.81704100
H	9.30857400	5.78495500	-0.55075700
C	5.84169600	0.40920300	-0.54152200
O	5.75190800	1.02450800	-1.57809500
O	6.13132300	0.93069300	0.65805800

Model3 with two target molecules arranged in parallel



E(UB3LYP) = -4024.29986226a.u.

C	9.90553300	-1.95043800	1.10357700
C	9.22581100	-2.58421100	0.06668200
C	7.83010800	-2.38595800	-0.11355100
C	7.15046700	-1.50561100	0.76670000
C	7.82916600	-0.90006500	1.85573900
C	9.22477200	-1.13081900	1.99934300
C	7.10220700	-0.12621300	2.79673400
C	5.67779600	-0.04423900	2.77019300
C	4.95980200	-0.64087800	1.69447300
C	5.70817700	-1.12503600	0.46955400
C	3.56214300	-0.69528200	1.71777700
C	2.84212700	-0.05109100	2.77098100
C	3.55737600	0.61395200	3.81833500
C	4.96089300	0.57751700	3.80725600
C	2.82061500	1.27172900	4.84424900
C	1.43948000	1.28942000	4.85614300
C	0.71019000	0.61597300	3.80805300
C	1.42191500	-0.05661900	2.77534500
C	4.95779300	-2.19982900	-0.28902500
C	5.67715000	-3.06711300	-1.15859400
C	7.10016500	-3.08865900	-1.10908800
C	3.56168900	-2.23530700	-0.24150200
C	2.83353000	-1.43778200	0.71601200
C	1.43468300	-1.47495500	0.74533000

C	0.70742200	-0.74798000	1.75112900
C	-0.70174600	-0.74804100	1.75182500
C	-1.41499300	-0.05645800	2.77636600
C	-0.70251300	0.61612600	3.80825800
C	4.95895200	-3.91820700	-2.01975600
C	3.55671600	-3.93596900	-2.04058900
C	2.84008700	-3.09458400	-1.12721900
C	1.42220800	-3.10240600	-1.12015700
C	0.70717900	-2.27814000	-0.19904900
C	-0.70254400	-2.27854200	-0.19851100
C	-1.43042200	-1.47503400	0.74641300
C	-2.83572300	-0.05057000	2.77256400
C	-3.55777500	-0.69446300	1.72047600
C	-2.82827800	-1.43819900	0.71768400
C	0.70794600	-3.93758300	-2.02728000
C	1.43698800	-4.78298000	-2.94226100
C	2.81925500	-4.76908900	-2.92882100
C	-0.70327000	-3.93782900	-2.02683500
C	-1.41773600	-3.10277600	-1.11885300
C	-2.83549500	-3.09534100	-1.12461600
C	-3.55777400	-2.23623500	-0.23820400
C	-4.95390100	-2.19915000	-0.28547100
C	-5.70418900	-1.11849900	0.46860600
C	-4.95422500	-0.63744800	1.69617800
C	-1.43057200	1.29085500	4.85718100
C	-0.67265200	1.95817600	5.89187700
C	0.68307300	1.95741700	5.89141100
C	-3.54895500	0.61718500	3.81976400
C	-2.81100200	1.27490200	4.84576800
C	-5.67071700	-0.03719400	2.77263000
C	-4.95120800	0.58416100	3.80880100
C	-7.14579500	-1.50676900	0.77356400
C	-7.82123900	-0.90745400	1.86201400
C	-7.09264300	-0.11413000	2.80239500
C	-9.20480300	-1.15477700	2.02330200

C	-9.88567400	-1.98646500	1.13947500
C	-9.20536700	-2.61170900	0.09770300
C	-7.82239000	-2.39185500	-0.09532700
C	-7.09055200	-3.09395800	-1.10826700
C	-5.67393700	-3.06934000	-1.15576000
C	-4.95248900	-3.92021800	-2.01888800
C	-3.55170800	-3.93699300	-2.03910800
C	-2.81400600	-4.76982600	-2.92792500
C	-1.43188400	-4.78341900	-2.94169200
C	0.68094300	-5.62017200	-3.84435700
C	-0.67581500	-5.62033000	-3.84409400
H	10.97324900	-2.11199500	1.22561000
H	9.75149300	-0.66462900	2.82790700
H	7.63709500	0.33845600	3.62117200
H	5.50940100	1.04240300	4.62348400
H	3.36966400	1.77290300	5.63860400
H	1.23439900	2.46398600	6.67985900
H	-1.22294800	2.46536200	6.68064000
H	-3.35964200	1.77717200	5.63969200
H	-5.49868900	1.05077100	4.62475900
H	-7.62910900	0.35403400	3.62335100
H	-9.72862800	-0.69356200	2.85667700
H	-10.94934700	-2.16349800	1.27374500
H	-9.73024500	-3.28737100	-0.57263200
H	-7.63127700	-3.74787400	-1.78700200
H	-5.50078900	-4.57782500	-2.68950200
H	-3.36241100	-5.40863900	-3.61682600
H	-1.22612900	-6.25726500	-4.53232300
H	1.23115500	-6.25698800	-4.53277600
H	3.36742900	-5.40811200	-3.61772600
H	5.50737900	-4.57574100	-2.69037600
H	7.63743000	-3.74485600	-1.78886600
H	9.75359100	-3.25006000	-0.61089900
O	6.97293800	5.53333100	-3.32385000
N	6.75365000	4.47405100	-2.63063700

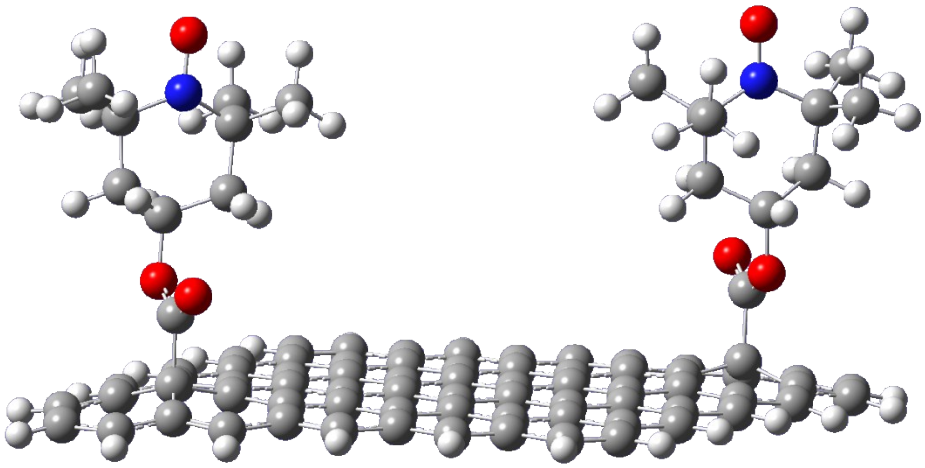
C	5.37296000	4.35521100	-2.04711300
C	5.16135700	2.94095800	-1.46478800
H	4.25220500	2.94695600	-0.85252100
H	5.00780600	2.22741900	-2.27854500
C	6.35349100	2.48478400	-0.63067000
H	6.51403000	3.17662700	0.19995900
C	7.60484000	2.41190100	-1.49862600
H	8.45249100	2.04256500	-0.90970200
H	7.42960900	1.69877400	-2.30856700
C	7.97842300	3.78852500	-2.09137200
C	4.37609400	4.58081300	-3.19594200
H	4.49774900	5.57968300	-3.61874500
H	4.53333200	3.84656600	-3.99260800
H	3.35230600	4.47185800	-2.82172400
C	5.17728800	5.45519400	-0.98149000
H	4.12858100	5.48819000	-0.66589200
H	5.79046100	5.29271000	-0.08943600
H	5.44487100	6.42525800	-1.40943200
C	8.65083700	4.70370900	-1.04537100
H	8.05996500	4.80150000	-0.12920100
H	9.63175300	4.30019800	-0.77034400
H	8.78985100	5.70081700	-1.47210500
C	8.93818100	3.58326100	-3.27498800
H	8.46252800	2.98286900	-4.05726900
H	9.83686100	3.05822300	-2.93300400
H	9.22693900	4.54386000	-3.70538300
C	5.85363600	0.09753000	-0.55969300
O	5.79572700	-0.03461400	-1.75964100
O	6.09428900	1.24282600	0.09285500
O	-6.99964300	5.52433900	-3.33153200
N	-6.77513500	4.46712400	-2.63679700
C	-7.99664500	3.77521800	-2.09822100
C	-7.61595400	2.40175000	-1.50286100
H	-8.46237500	2.02844700	-0.91464300
H	-7.43538900	1.68824800	-2.31133700

C	-6.36634200	2.48273700	-0.63303700
H	-6.53211200	3.17543700	0.19591800
C	-5.17576300	2.94492400	-1.46635600
H	-4.26749300	2.95710800	-0.85284200
H	-5.01694500	2.23106400	-2.27874200
C	-5.39465400	4.35704000	-2.05103900
C	-8.95361400	3.56276200	-3.28283900
H	-9.24703900	4.52101200	-3.71532900
H	-8.47360200	2.96361300	-4.06341500
H	-9.84988700	3.03339800	-2.94118800
C	-8.67571900	4.68823800	-1.05458800
H	-9.65455800	4.27937600	-0.78002000
H	-8.08654900	4.79110600	-0.13787000
H	-8.82015200	5.68375500	-1.48324600
C	-5.20696700	5.45979000	-0.98682900
H	-5.82052600	5.29507000	-0.09546300
H	-4.15893700	5.49926500	-0.66969800
H	-5.47945800	6.42768100	-1.41660700
C	-4.39744200	4.58680400	-3.19874900
H	-4.54927700	3.85047300	-3.99453600
H	-3.37358100	4.48426500	-2.82290000
H	-4.52419900	5.58434300	-3.62321800
C	-5.85079500	0.09829100	-0.55822500
O	-5.78696000	-0.03242700	-1.75856000
O	-6.10177600	1.24375600	0.09242100

==========

(4) Model4

Model4 with two target molecules arranged in opposite direction



E(UB3LYP) = -4024.36584076a.u.

O	-6.77999000	6.38385800	-0.31461500
N	-6.86662000	5.10304700	-0.26345900
C	-5.56255700	4.35996600	-0.35918300
C	-5.77448800	2.86520900	-0.03551300
H	-4.87696500	2.31272100	-0.33638300
H	-5.89577500	2.73745800	1.04336500
C	-7.00189700	2.29483800	-0.73756100
H	-6.89056500	2.38882800	-1.82077100
C	-8.25847700	3.02512500	-0.27661200
H	-9.14472500	2.58774300	-0.75103200
H	-8.36381900	2.89460800	0.80347500
C	-8.21179500	4.53085500	-0.61617500
C	-4.61720400	4.97175300	0.68793800
H	-4.44232400	6.02812900	0.47619800
H	-5.04715400	4.88658600	1.69120400
H	-3.65968600	4.43979700	0.67483800
C	-4.96389000	4.56780200	-1.76694900
H	-3.94348900	4.17038500	-1.80193800
H	-5.54402800	4.06927400	-2.54986600
H	-4.93077000	5.63722600	-1.99256900
C	-8.49749300	4.79668200	-2.11004000
H	-7.85145700	4.21337800	-2.77360800
H	-9.53709000	4.54154100	-2.34423300

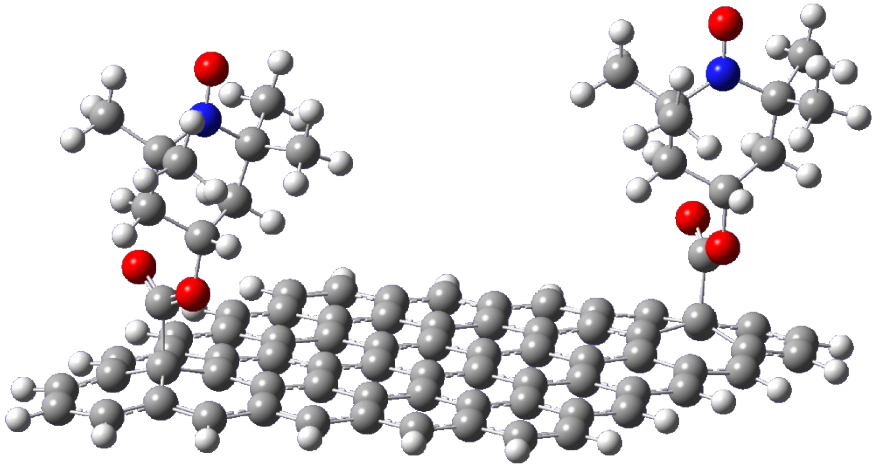
H	-8.34068100	5.85727200	-2.32487600
C	-9.25482100	5.27184700	0.23692400
H	-9.03790000	5.14940900	1.30295600
H	-10.25163100	4.86373600	0.03682200
H	-9.25207600	6.33847700	0.00519900
C	-7.22799500	0.27479900	0.60989200
O	-7.32147600	0.86500200	1.66103500
O	-7.10644700	0.84469900	-0.59702000
O	6.77912000	6.38438300	0.30729300
N	6.86591100	5.10352600	0.25761200
C	5.56197000	4.36037400	0.35438700
C	5.77405000	2.86530200	0.03225500
H	4.87664200	2.31302900	0.33385900
H	5.89518900	2.73640000	-1.04650300
C	7.00163100	2.29587800	0.73476000
H	6.89042000	2.39107800	1.81787100
C	8.25806300	3.02581600	0.27284300
H	9.14442700	2.58907200	0.74763300
H	8.36329900	2.89413800	-0.80711500
C	8.21121500	4.53191600	0.61076700
C	4.61631600	4.97093400	-0.69317500
H	4.44137400	6.02752000	-0.48253600
H	5.04604000	4.88472900	-1.69644900
H	3.65885200	4.43889700	-0.67927700
C	4.96358200	4.56960400	1.76206900
H	3.94321300	4.17216200	1.79769000
H	5.54392400	4.07190800	2.54536600
H	4.93044300	5.63925300	1.98661300
C	8.49709800	4.79941300	2.10429800
H	7.85123200	4.21676600	2.76860700
H	9.53675900	4.54465100	2.33861600
H	8.34020300	5.86022200	2.31798300
C	9.25401100	5.27213000	-0.24328800
H	9.03696500	5.14848300	-1.30915400
H	10.25091500	4.86440100	-0.04286800

H	9.25112700	6.33901600	-0.01273900
C	7.22800500	0.27428900	-0.61034500
O	7.32142100	0.86326100	-1.66218400
O	7.10633600	0.84557900	0.59587900
C	9.90631300	-2.09831500	-0.66859700
C	9.14156600	-2.07642300	-1.83636900
C	7.74604800	-1.83572600	-1.80350800
C	7.14976600	-1.31370600	-0.49918600
C	7.92477600	-1.75502800	0.74045300
C	9.31614200	-1.98587300	0.59178400
C	7.27685800	-1.85593900	1.94880600
C	5.85175900	-1.73697000	2.08874600
C	5.04978900	-1.66059500	0.87996700
C	5.65697000	-1.59749000	-0.38587800
C	3.63209100	-1.70690600	0.98494100
C	3.00311600	-1.73538200	2.26743100
C	3.80285600	-1.76383900	3.45536000
C	5.22388800	-1.78530800	3.31867700
C	3.16202900	-1.79082100	4.70567500
C	1.76678600	-1.79051800	4.82505300
C	0.96211800	-1.76493500	3.64155000
C	1.59003000	-1.74000400	2.36565700
C	4.88256300	-1.68088600	-1.55599000
C	5.51300500	-1.78924600	-2.86027500
C	6.94105000	-1.94343200	-2.91147000
C	3.46397400	-1.71997200	-1.46704200
C	2.83859100	-1.70520700	-0.19258300
C	1.41447900	-1.71701100	-0.09546000
C	0.79103900	-1.72372400	1.17958700
C	-0.62338100	-1.72544900	1.27595200
C	-1.25369800	-1.74729300	2.55954800
C	-0.45853800	-1.77008000	3.73822800
C	4.72424800	-1.84056000	-3.99341700
C	3.29838800	-1.79817800	-3.93680000
C	2.66711200	-1.75468500	-2.65181100

C	1.25392300	-1.75058600	-2.55752500
C	0.62360700	-1.72706700	-1.27395900
C	-0.79081400	-1.72524600	-1.17759500
C	-1.41425400	-1.71684700	0.09744200
C	-2.66688600	-1.75130500	2.65383700
C	-3.46374900	-1.71809500	1.46902600
C	-2.83836600	-1.70495200	0.19454900
C	0.45876300	-1.77486900	-3.73617500
C	1.09548900	-1.80968300	-5.01779000
C	2.49394600	-1.82400900	-5.08856900
C	-0.96189400	-1.76961000	-3.63950200
C	-1.58980500	-1.74301000	-2.36364400
C	-3.00289200	-1.73827900	-2.26542300
C	-3.63186600	-1.70814500	-0.98297200
C	-5.04957000	-1.66175000	-0.87805900
C	-5.65675200	-1.59707000	0.38770500
C	-4.88234100	-1.67896200	1.55792300
C	-1.09526500	-1.80325200	5.01988700
C	-0.26092500	-1.82614700	6.19079100
C	1.09906600	-1.81960400	6.09829400
C	-3.29816300	-1.79319100	3.93888000
C	-2.49372100	-1.81752100	5.09068200
C	-5.51277700	-1.78576500	2.86234000
C	-4.72401900	-1.83559700	3.99554700
C	-7.14958300	-1.31330200	0.50066000
C	-7.74581200	-1.83378600	1.80562800
C	-6.94080200	-1.94003800	2.91372300
C	-9.14129900	-2.07458300	1.83879100
C	-9.90605300	-2.09798600	0.67104600
C	-9.31590100	-1.98703900	-0.58946800
C	-7.92454700	-1.75625200	-0.73842700
C	-7.27662500	-1.85863100	-1.94664400
C	-5.85153500	-1.73972700	-2.08673900
C	-5.22366300	-1.78962100	-3.31660500
C	-3.80263100	-1.76828200	-3.45331400

C	-3.16180500	-1.79687900	-4.70359300
C	-1.76656200	-1.79672300	-4.82297100
C	0.26114800	-1.83410600	-6.18866300
C	-1.09884400	-1.82745700	-6.09617400
H	10.97354400	-2.29103200	-0.73804000
H	9.91325200	-2.14786300	1.48580900
H	7.85929500	-2.07519000	2.84178200
H	5.82816800	-1.85528000	4.22074100
H	3.76917100	-1.81519600	5.60823700
H	1.70845500	-1.83829200	6.99861400
H	-0.74245100	-1.85010200	7.16532600
H	-2.97291400	-1.84986700	6.06688100
H	-5.20019700	-1.92425700	4.96963600
H	-7.39193300	-2.18654000	3.87280600
H	-9.60740600	-2.29171500	2.79648900
H	-10.97326600	-2.29071600	0.74073400
H	-9.91300400	-2.15017200	-1.48328900
H	-7.85904300	-2.07906800	-2.83934200
H	-5.82793500	-1.86080300	-4.21857900
H	-3.76894600	-1.82244900	-5.60612200
H	-1.70823300	-1.84732400	-6.99646800
H	0.74267400	-1.85932200	-7.16316700
H	2.97313900	-1.85758500	-6.06472700
H	5.20043100	-1.93039200	-4.96739700
H	7.39220500	-2.19105600	-3.87025200
H	9.60770000	-2.29466500	-2.79380200

Model4 with two target molecules arranged in parallel



E(UB3LYP) = -4024.36586123a.u.

O	-6.87145400	5.38968800	-3.48129100
N	-6.93640500	4.33752100	-2.74686900
C	-8.25882600	4.10064000	-2.07223600
C	-8.28805000	2.69766300	-1.42692700
H	-9.15029500	2.64184600	-0.75221700
H	-8.42451800	1.93790000	-2.20072800
C	-7.00285400	2.39441600	-0.66501700
H	-6.85548900	3.13249600	0.12745600
C	-5.81309200	2.41008000	-1.61797900
H	-4.89584700	2.14351700	-1.08051400
H	-5.97326400	1.65555900	-2.39300000
C	-5.61656300	3.79461400	-2.27303400
C	-9.34103500	4.17601400	-3.16222600
H	-9.35043700	5.16414800	-3.62581600
H	-9.15515600	3.43049800	-3.94215100
H	-10.32373800	3.97780300	-2.72038400
C	-8.50415800	5.21751800	-1.03482100
H	-9.53070400	5.15806600	-0.65617400
H	-7.82639800	5.15220400	-0.17778800
H	-8.36231100	6.19158400	-1.51084400
C	-4.97298900	4.80702000	-1.30106100
H	-5.51758800	4.88843300	-0.35503500
H	-3.94550500	4.50404000	-1.07101800
H	-4.95025100	5.79479700	-1.76953400

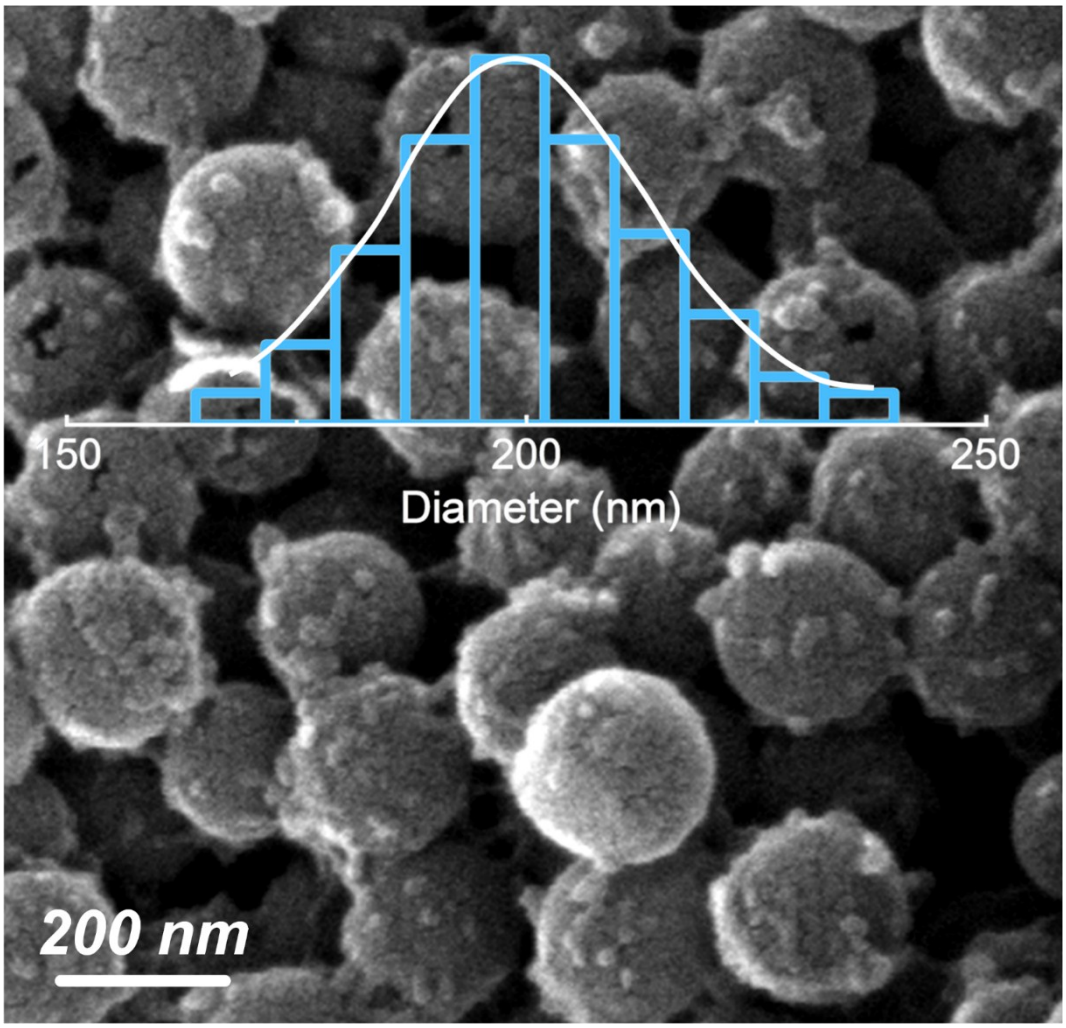
C	-4.71927000	3.64334200	-3.51248200
H	-5.18095600	2.97169700	-4.24348600
H	-3.75177500	3.22245600	-3.21794800
H	-4.55748500	4.61209700	-3.98868700
C	-7.25715200	-0.02470900	-0.47396700
O	-7.40200900	-0.20700300	-1.66038200
O	-7.08265800	1.16499500	0.11758600
O	6.87182800	5.38945600	-3.48143500
N	6.93670200	4.33731600	-2.74697300
C	5.61680200	3.79451300	-2.27317100
C	5.81320400	2.41002100	-1.61800900
H	4.89591700	2.14355000	-1.08056800
H	5.97338900	1.65541400	-2.39294900
C	7.00290700	2.39436400	-0.66497200
H	6.85552500	3.13248300	0.12746100
C	8.28816500	2.69749800	-1.42681700
H	9.15036500	2.64167900	-0.75204800
H	8.42464600	1.93768200	-2.20056300
C	8.25905900	4.10042900	-2.07223800
C	4.71956600	3.64321700	-3.51265700
H	4.55781600	4.61194700	-3.98892600
H	5.18127600	2.97152900	-4.24360500
H	3.75204900	3.22236100	-3.21815000
C	4.97321900	4.80701900	-1.30130400
H	3.94570200	4.50409800	-1.07132500
H	5.51774000	4.88846100	-0.35523500
H	4.95054800	5.79476500	-1.76984900
C	8.50440200	5.21738900	-1.03491600
H	7.82658400	5.15221900	-0.17791700
H	9.53092100	5.15791100	-0.65619600
H	8.36265500	6.19141700	-1.51105000
C	9.34134300	4.17564600	-3.16216700
H	9.15542800	3.43011300	-3.94206900
H	10.32399700	3.97736200	-2.72025400
H	9.35086900	5.16375400	-3.62581600

C	7.25706400	-0.02474100	-0.47388500
O	7.40207100	-0.20701700	-1.66028400
O	7.08256300	1.16496600	0.11765100
C	9.92881000	-1.81228900	1.09739100
C	9.24692300	-2.54835500	0.12693900
C	7.85226500	-2.39834500	-0.07229400
C	7.16823400	-1.20664500	0.59168200
C	7.85496800	-0.75454900	1.87873800
C	9.25251600	-0.97062500	1.98297400
C	7.12567100	-0.10845700	2.84863800
C	5.69550500	0.02037900	2.80032100
C	4.97816300	-0.70447900	1.76567000
C	5.67044200	-1.42053600	0.77415100
C	3.55649100	-0.73084400	1.79765400
C	2.84172300	0.02675400	2.77549200
C	3.55867400	0.78097200	3.75982100
C	4.98544400	0.72988000	3.74979000
C	2.83435000	1.52210800	4.70874800
C	1.43424000	1.54458500	4.72185100
C	0.71193800	0.78777800	3.74484400
C	1.42519100	0.02903300	2.77621000
C	4.97763800	-2.24976300	-0.12497600
C	5.69567400	-3.12130800	-1.03862600
C	7.12473400	-3.20683700	-0.91130900
C	3.55613300	-2.28655900	-0.10501700
C	2.84521000	-1.50144100	0.84038600
C	1.41768400	-1.50989700	0.84743200
C	0.70885000	-0.73799000	1.80458600
C	-0.70895400	-0.73798300	1.80456700
C	-1.42531300	0.02903000	2.77618400
C	-0.71207800	0.78777600	3.74483200
C	4.98559800	-3.90967800	-1.92356800
C	3.55886500	-3.90903500	-1.97583000
C	2.84158500	-3.09471000	-1.04112800
C	1.42514400	-3.09611900	-1.04250600

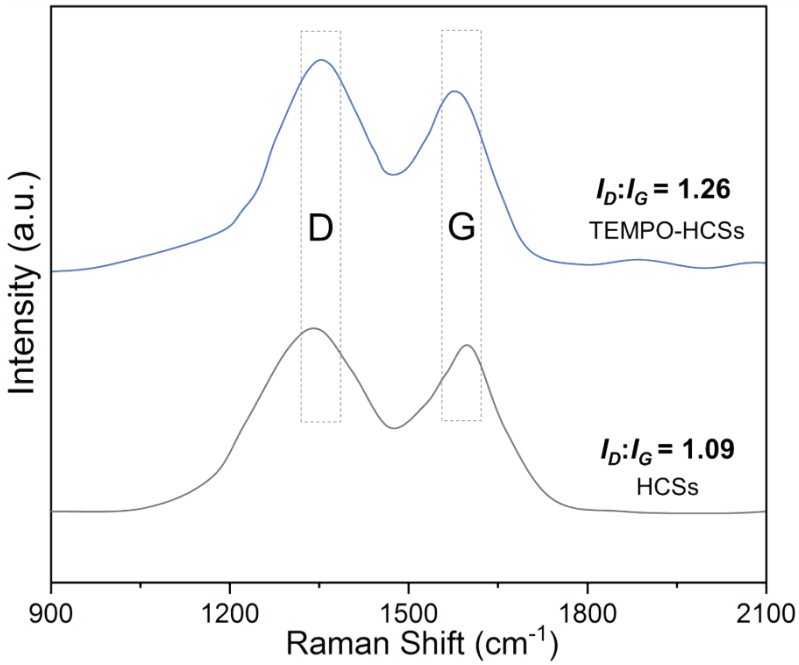
C	0.70884600	-2.29555000	-0.09846700
C	-0.70891300	-2.29554300	-0.09848600
C	-1.41776900	-1.50989600	0.84740300
C	-2.84184500	0.02675300	2.77543800
C	-3.55659400	-0.73084000	1.79757900
C	-2.84529400	-1.50143100	0.84032000
C	0.71198500	-3.89625800	-1.97703700
C	1.43442500	-4.70419100	-2.91207000
C	2.83454500	-4.69400300	-2.88891800
C	-0.71201800	-3.89625400	-1.97705500
C	-1.42519400	-3.09611200	-1.04253900
C	-2.84163600	-3.09469500	-1.04119400
C	-3.55620000	-2.28654700	-0.10509600
C	-4.97770600	-2.24974500	-0.12508400
C	-5.67053300	-1.42053000	0.77404000
C	-4.97826300	-0.70447800	1.76557400
C	-1.43439800	1.54457300	4.72183200
C	-0.68167600	2.29801500	5.68795100
C	0.68149900	2.29802300	5.68795900
C	-3.55881400	0.78095400	3.75976700
C	-2.83450700	1.52208600	4.70871100
C	-5.69562400	0.02034800	2.80023500
C	-4.98558200	0.72984600	3.74972200
C	-7.16830900	-1.20665300	0.59156000
C	-7.85507100	-0.75461900	1.87864000
C	-7.12578300	-0.10852700	2.84855300
C	-9.25260200	-0.97071600	1.98285300
C	-9.92889800	-1.81233100	1.09719900
C	-9.24701500	-2.54832500	0.12671500
C	-7.85233500	-2.39831700	-0.07248300
C	-7.12479500	-3.20679000	-0.91149300
C	-5.69572100	-3.12127500	-1.03876200
C	-4.98563100	-3.90964500	-1.92368700
C	-3.55889700	-3.90901400	-1.97591600
C	-2.83456000	-4.69398500	-2.88898700

C	-1.43444000	-4.70418000	-2.91210700
C	0.68158200	-5.50294900	-3.84109100
C	-0.68157900	-5.50294400	-3.84110800
H	10.99804500	-1.96174800	1.22126300
H	9.78609500	-0.52046900	2.81648500
H	7.64464600	0.29700800	3.71523400
H	5.52691600	1.26127300	4.52967800
H	3.37881200	2.09320500	5.45789600
H	1.22831000	2.87409300	6.43052500
H	-1.22850100	2.87407600	6.43051500
H	-3.37898300	2.09316100	5.45786600
H	-5.52706600	1.26119600	4.52963100
H	-7.64476600	0.29690100	3.71516100
H	-9.78619900	-0.52062100	2.81638600
H	-10.99813400	-1.96178600	1.22106200
H	-9.77779000	-3.29239000	-0.46169000
H	-7.64085700	-3.97684800	-1.48143400
H	-5.52678100	-4.56851500	-2.59934000
H	-3.37898500	-5.31348500	-3.59854800
H	-1.22819200	-6.11619000	-4.55338700
H	1.22820800	-6.11620200	-4.55335300
H	3.37898100	-5.31351500	-3.59845900
H	5.52675500	-4.56856600	-2.59919700
H	7.64081200	-3.97691300	-1.48121300
H	9.77771000	-3.29246300	-0.46140100

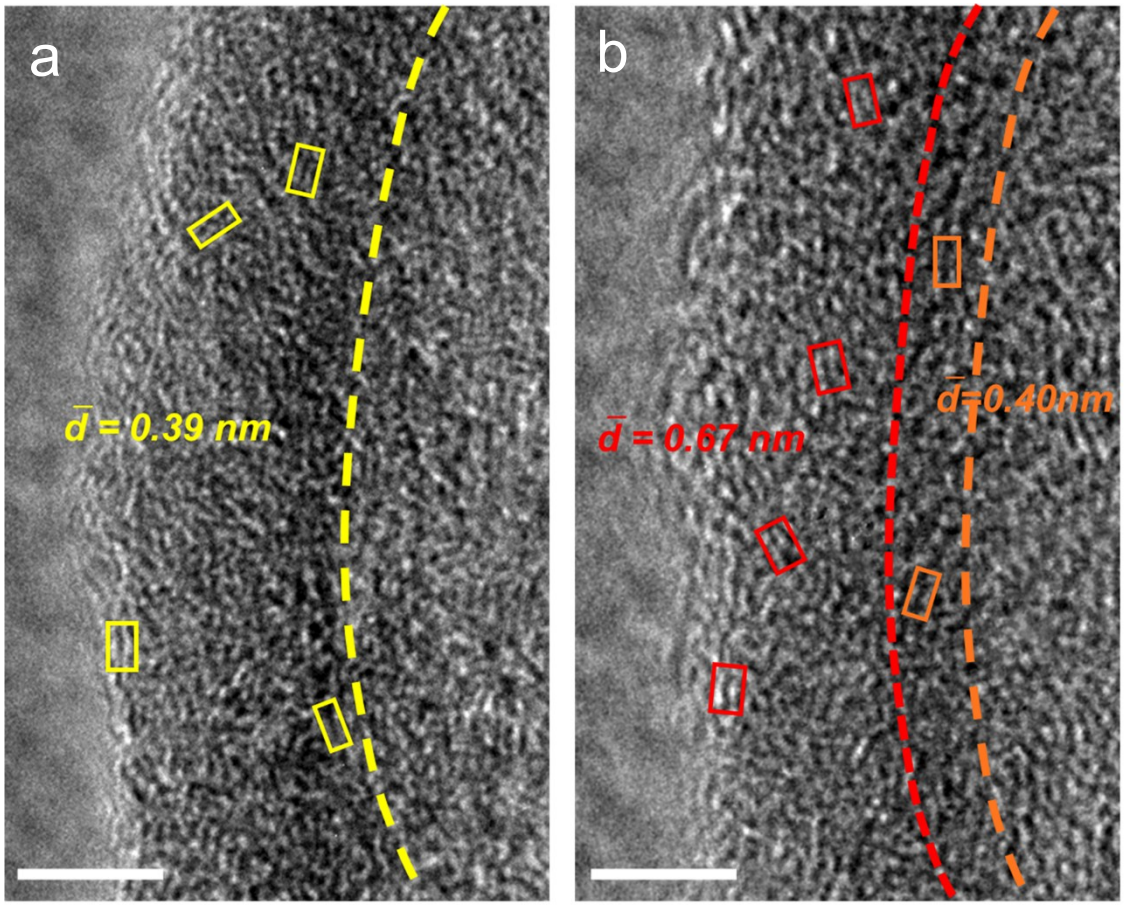
3. Supporting Figures



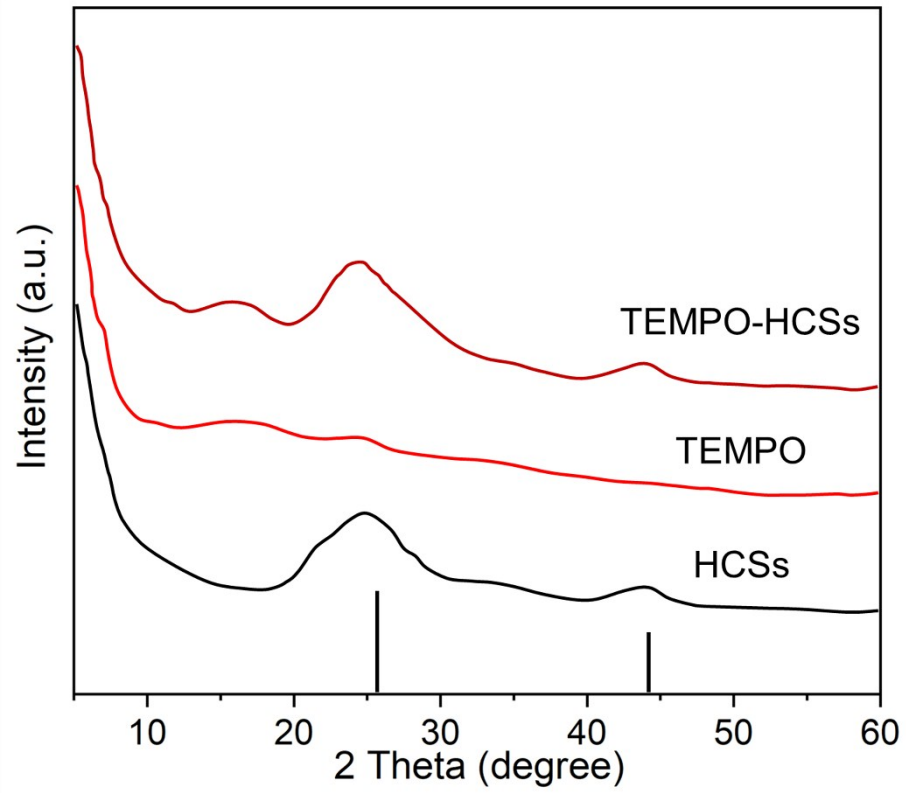
Supplementary Fig. S1 SEM image and size distribution of TEMPO–HCSs



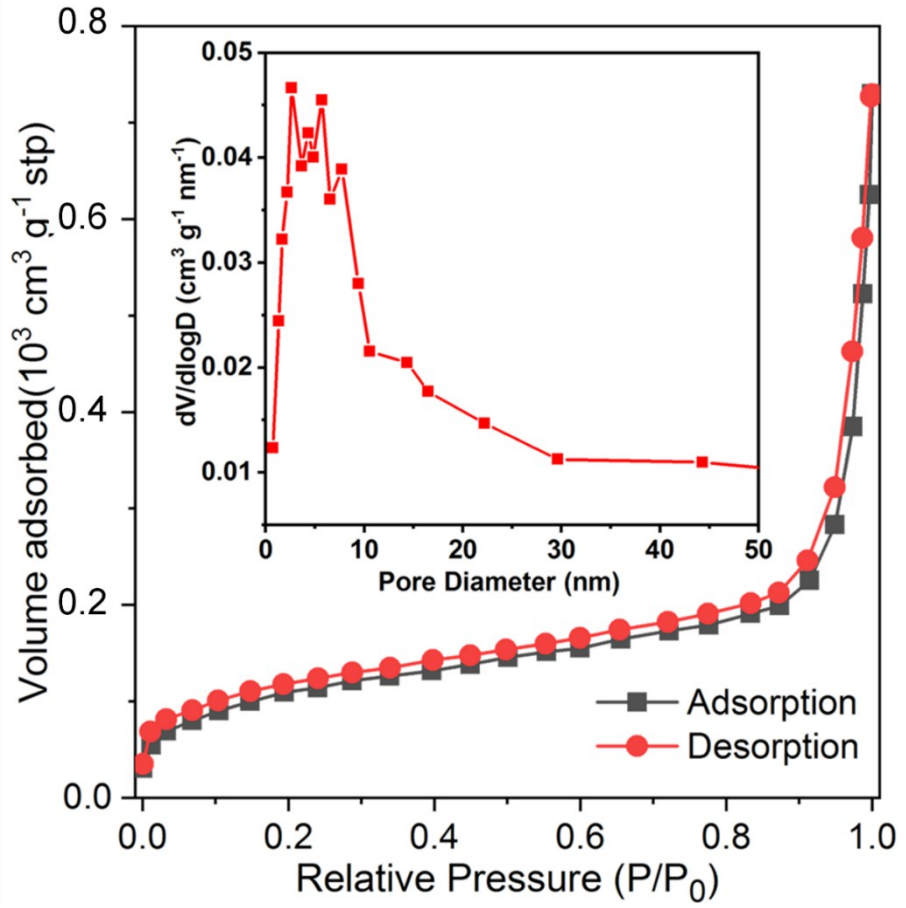
Supplementary Fig. S2 The Raman spectra of HCSs and TEMPO-HCSs at 900–2100 cm^{-1}.



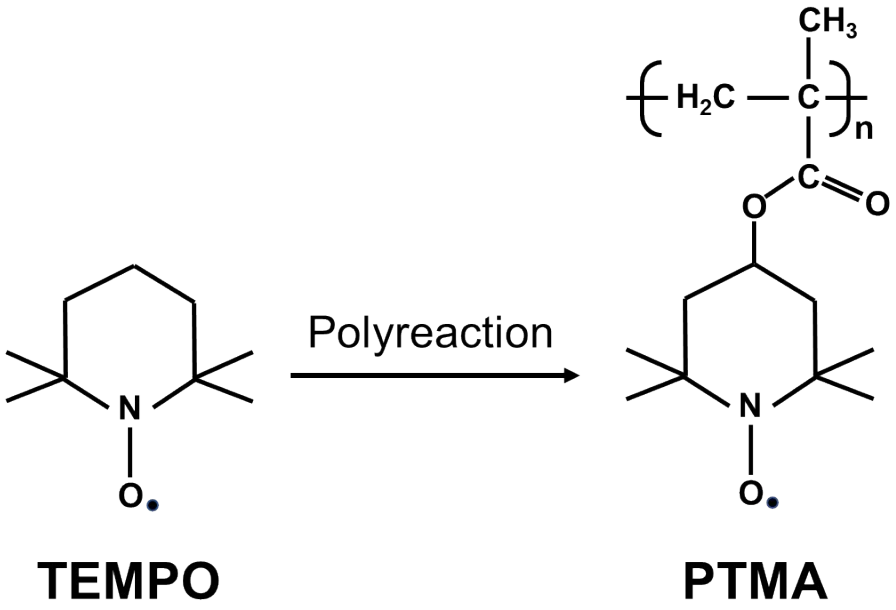
Supplementary Fig. S3 HRTEM images of HCSs and TEMPO-HCSs: a) HCSs; b) TEMPO-HCSs. The scale bar is 5 nm.



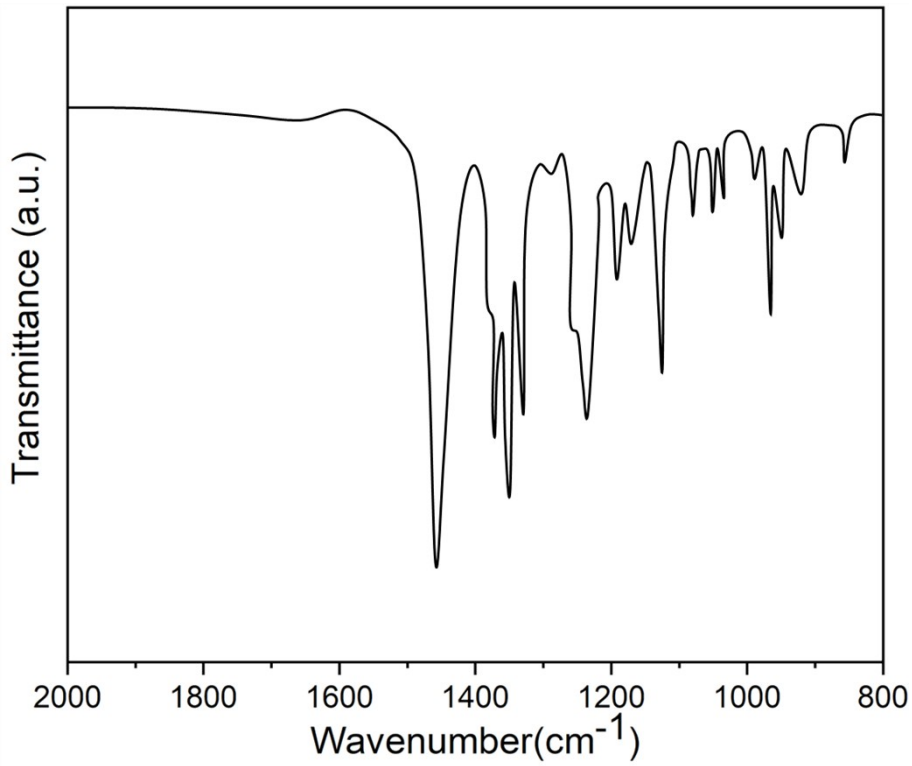
Supplementary Fig. S4 XRD pattern of HCSs,TEMPO and TEMPO-HCSs



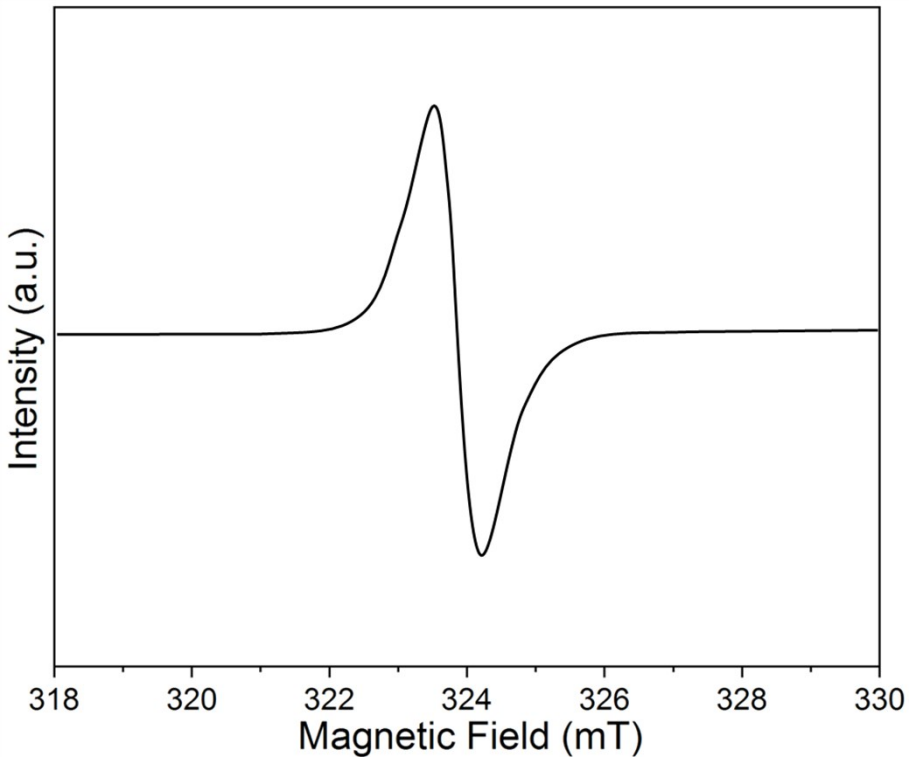
Supplementary Fig. S5 Nitrogen adsorption−desorption isotherms and pore size distribution of TEMPO-HCSs



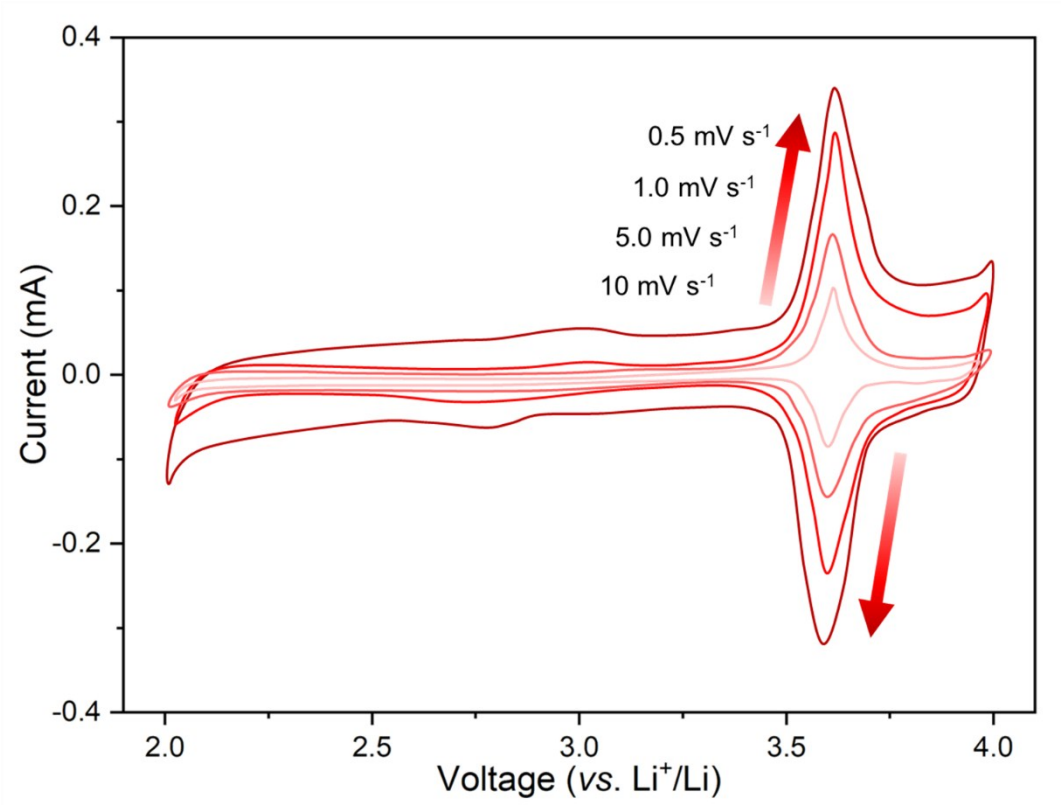
Supplementary Fig. S6 The radical polymer PTMA is prepared by the polymerization reaction of a small molecule radical compound TEMPO.



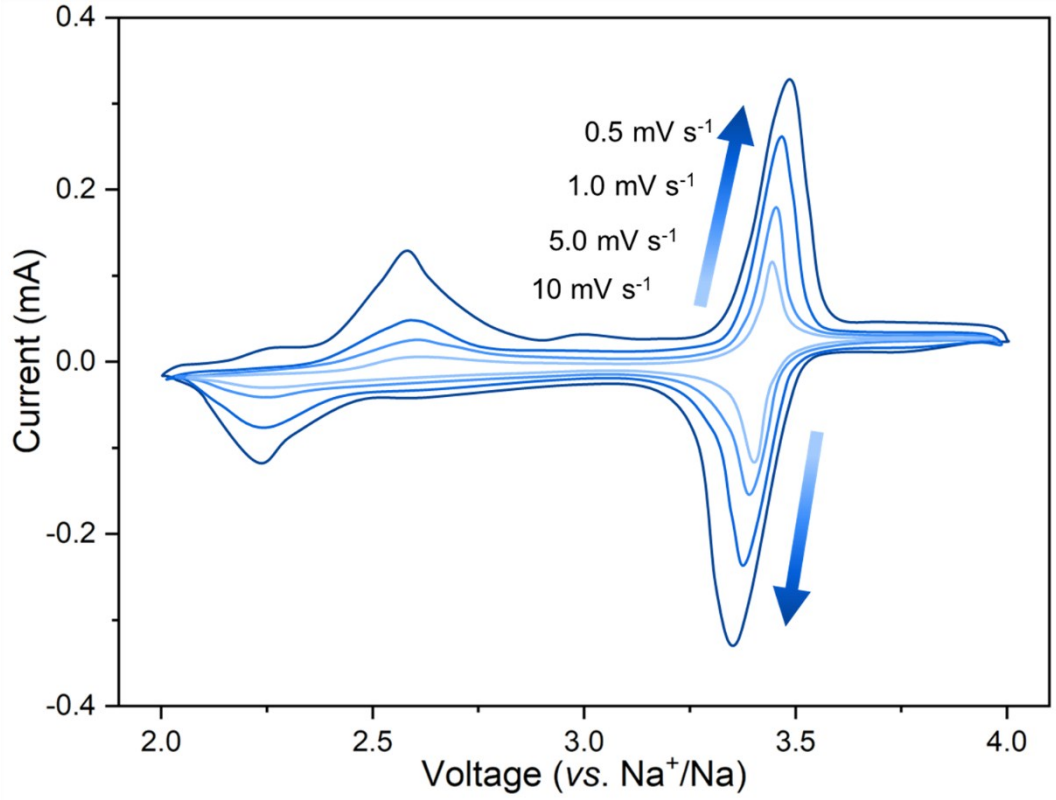
Supplementary Fig. S7 The Infrared spectra of TEMPO.



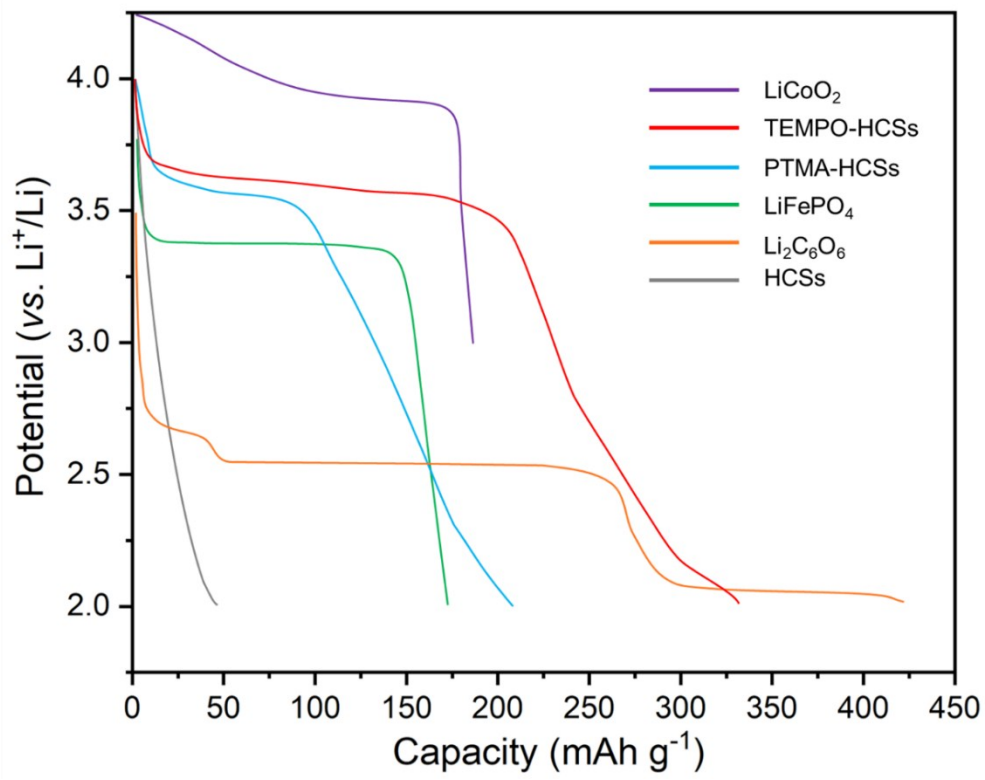
Supplementary Fig. S8 The Electron spin resonance (ESR) spectroscopy of TEMPO.



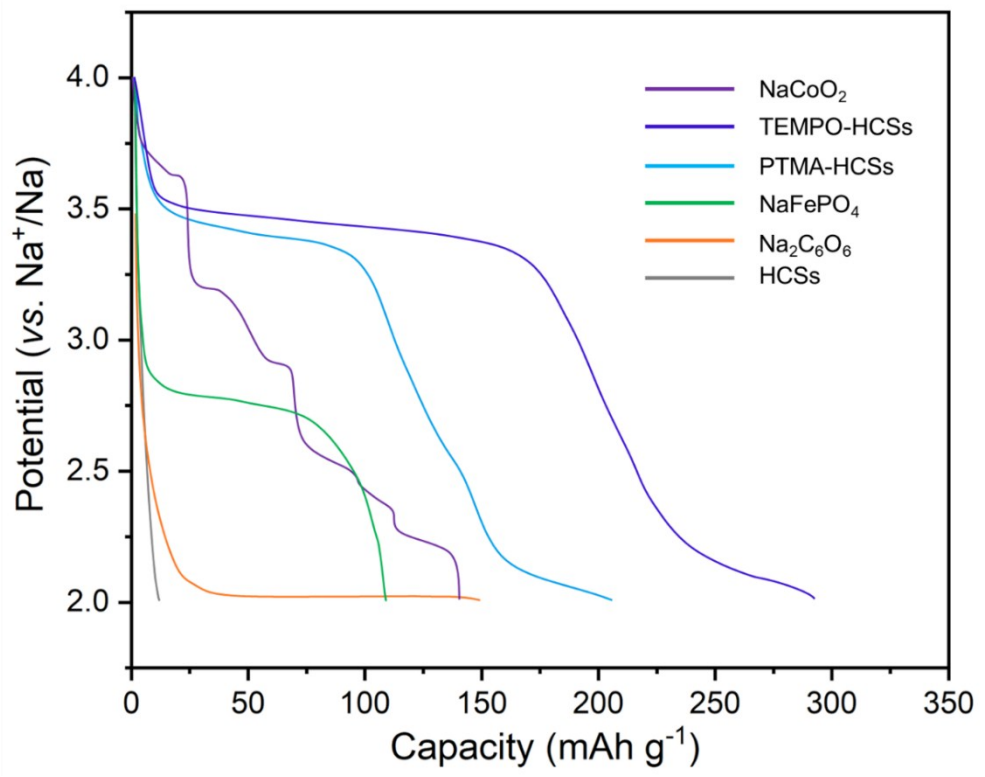
Supplementary Fig. S9 Cyclic voltammetry curves of the Li/TEMPO-HCSs at various voltage scan rates.



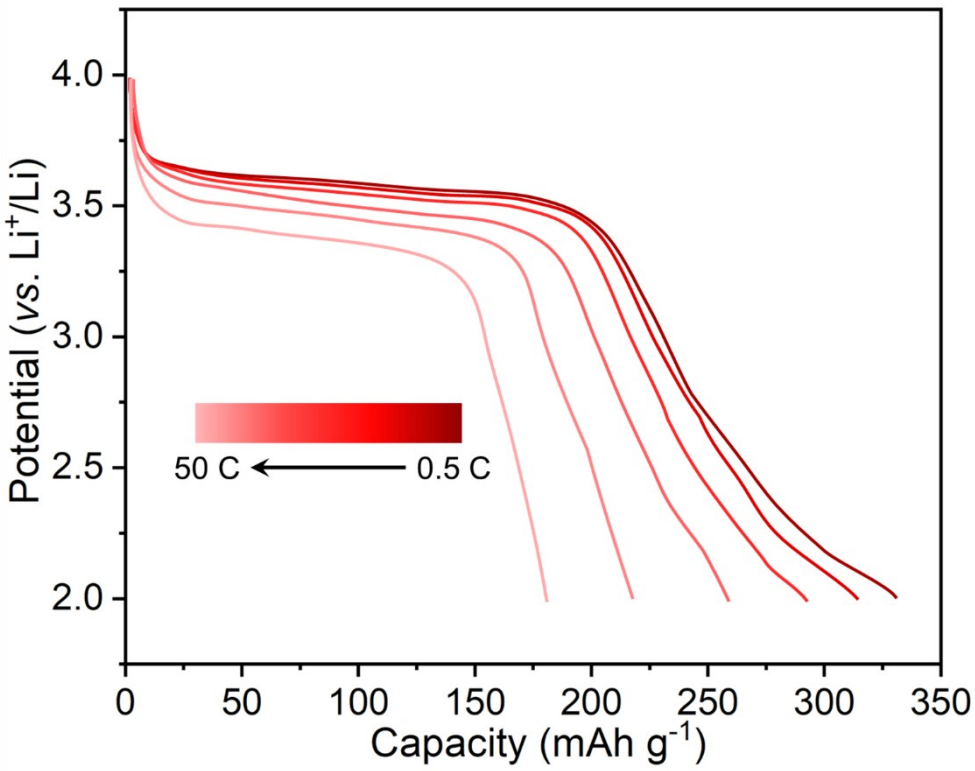
Supplementary Fig. S10 Cyclic voltammetry curves of the Na/TEMPO-HCSs at various voltage scan rates.



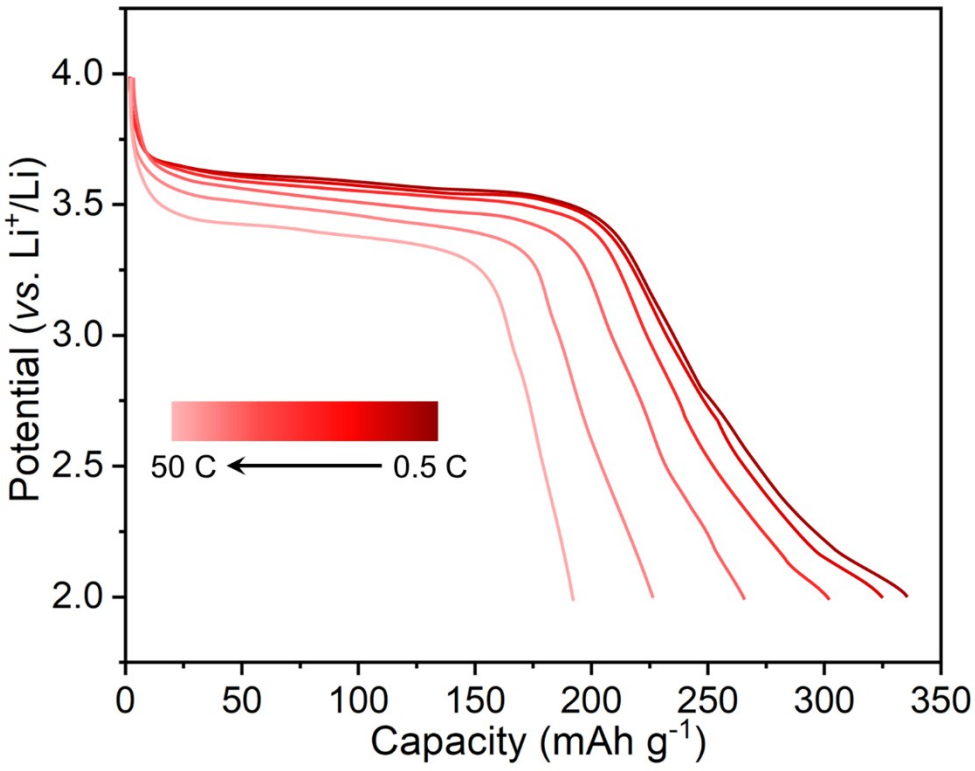
Supplementary Fig. S11 Initial discharge curves of different cathodes ($LiCoO_2$, TEMPO-HCSs, PTMA-HCSs, $LiFePO_4$, $Li_2C_6O_6$ and HCSs) at 0.5C in 0.1 MPa.



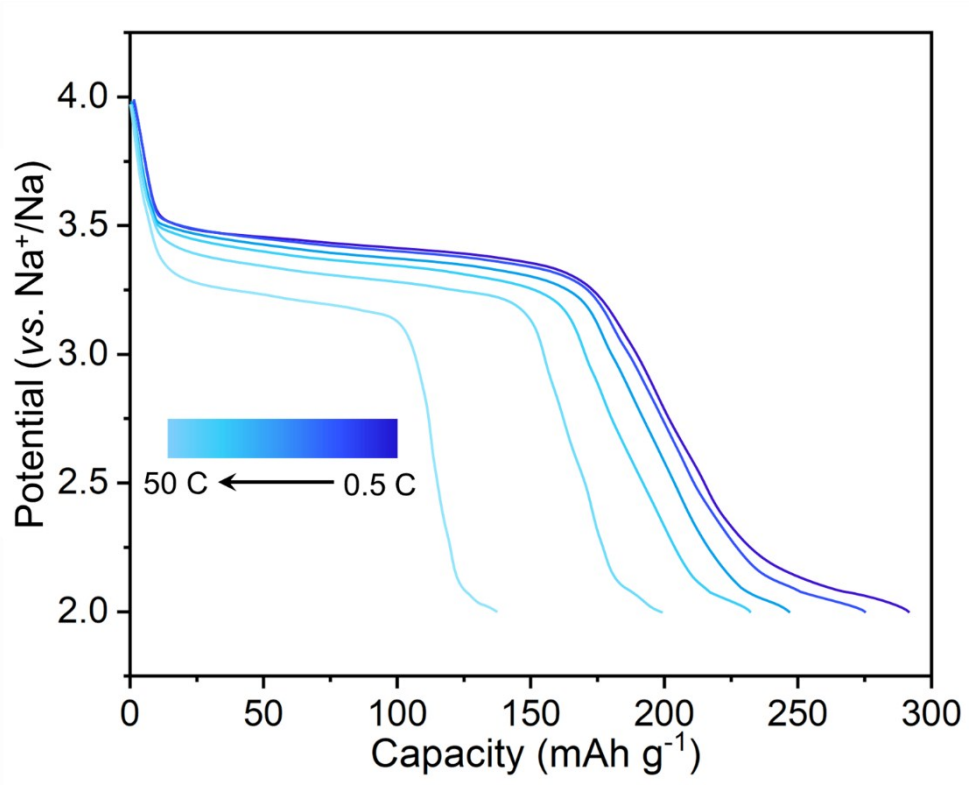
Supplementary Fig. S12 Initial discharge curves of different cathodes ($NaCoO_2$, TEMPO-HCSs, PTMA-HCSs, $NaFePO_4$, $Na_2C_6O_6$ and HCSs) at 0.5C in 0.1 MPa.



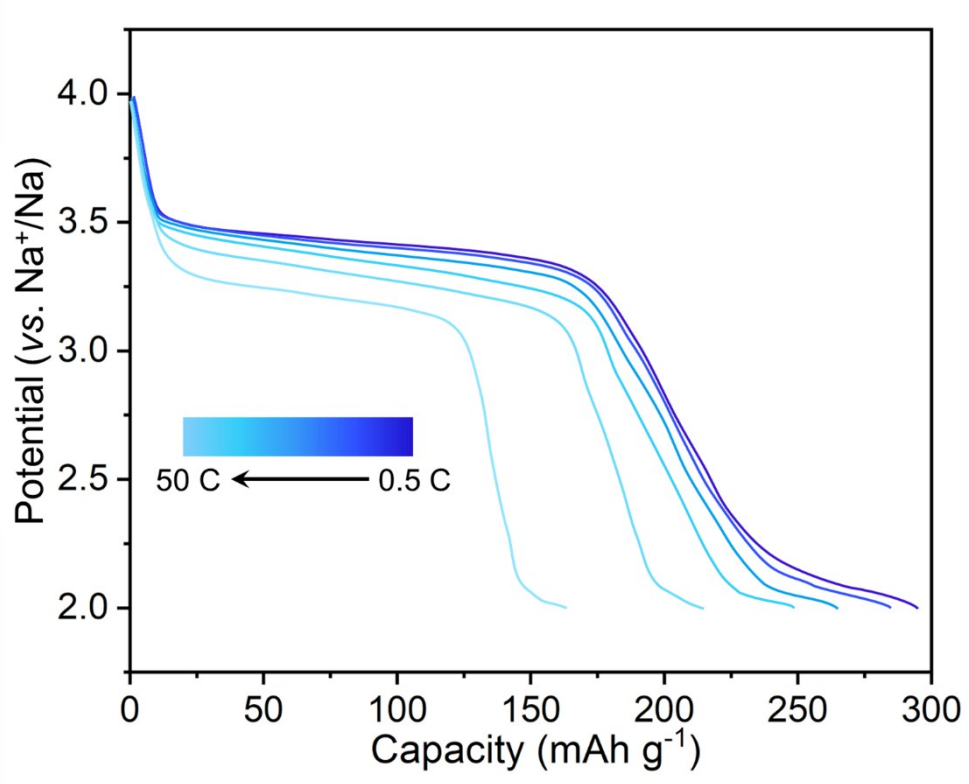
Supplementary Fig. S13 The discharge curves of Li/TEMPO-HCSs with different rates in 0.1 MPa.



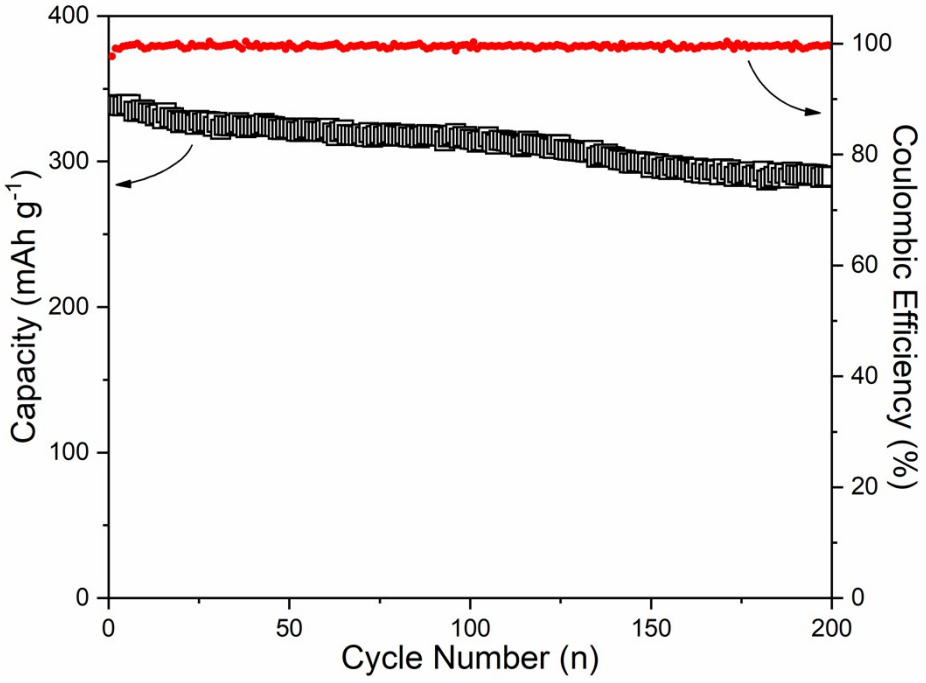
Supplementary Fig. S14 The discharge curves of Li/TEMPO-HCSs with different rates in 5.0 MPa.



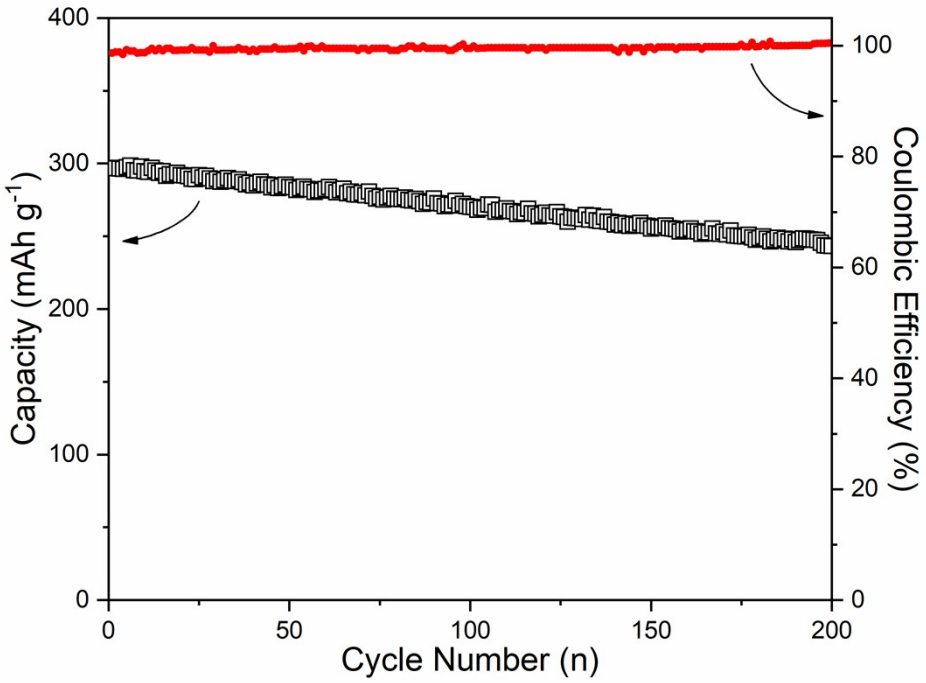
Supplementary Fig. S15 The discharge curves of Na/TEMPO-HCSs with different rates in 0.1 MPa.



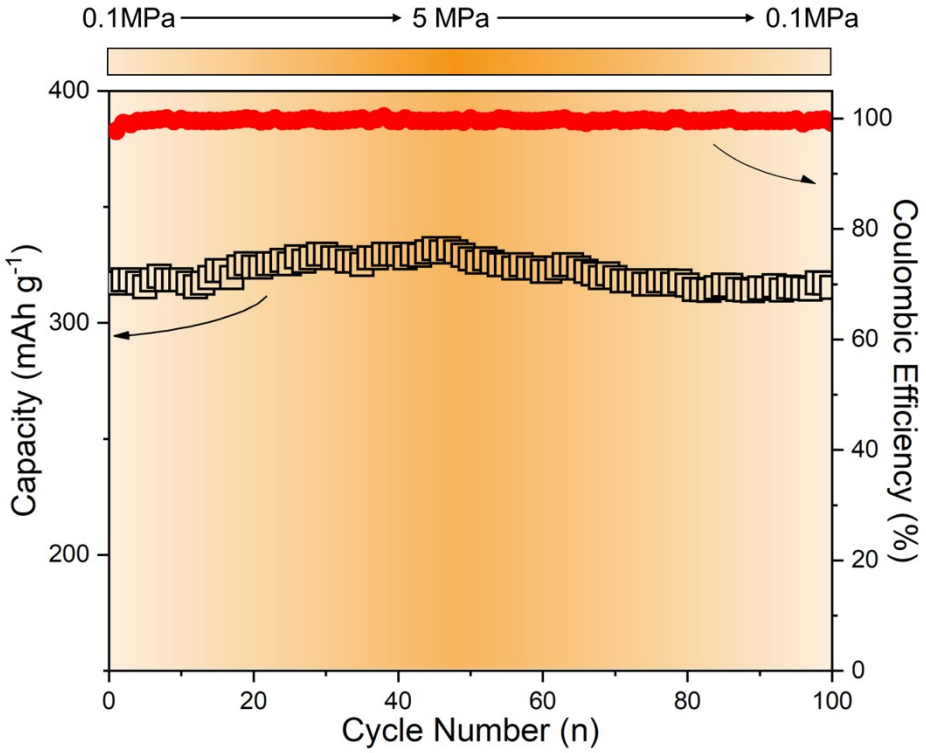
Supplementary Fig. S16 The discharge curves of Na/TEMPO-HCSs with different rates in 5.0 MPa.



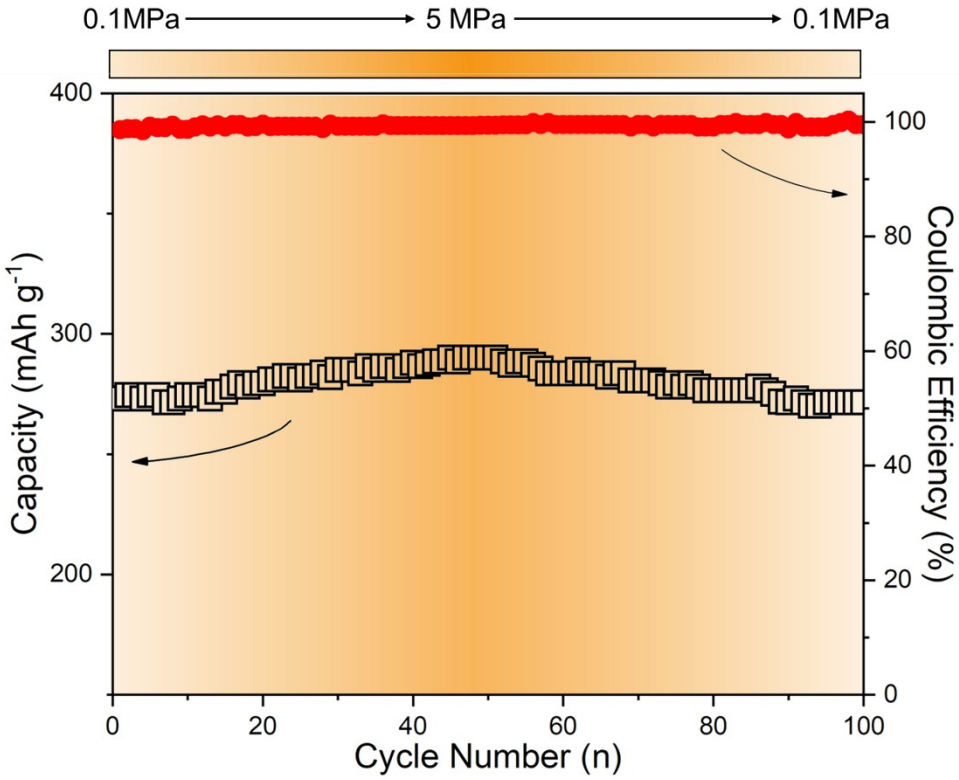
Supplementary Fig. S17 The Cycling profiles and columbic efficiency of Li/TEMPO-HCSs at 0.5 C in 5.0 MPa.



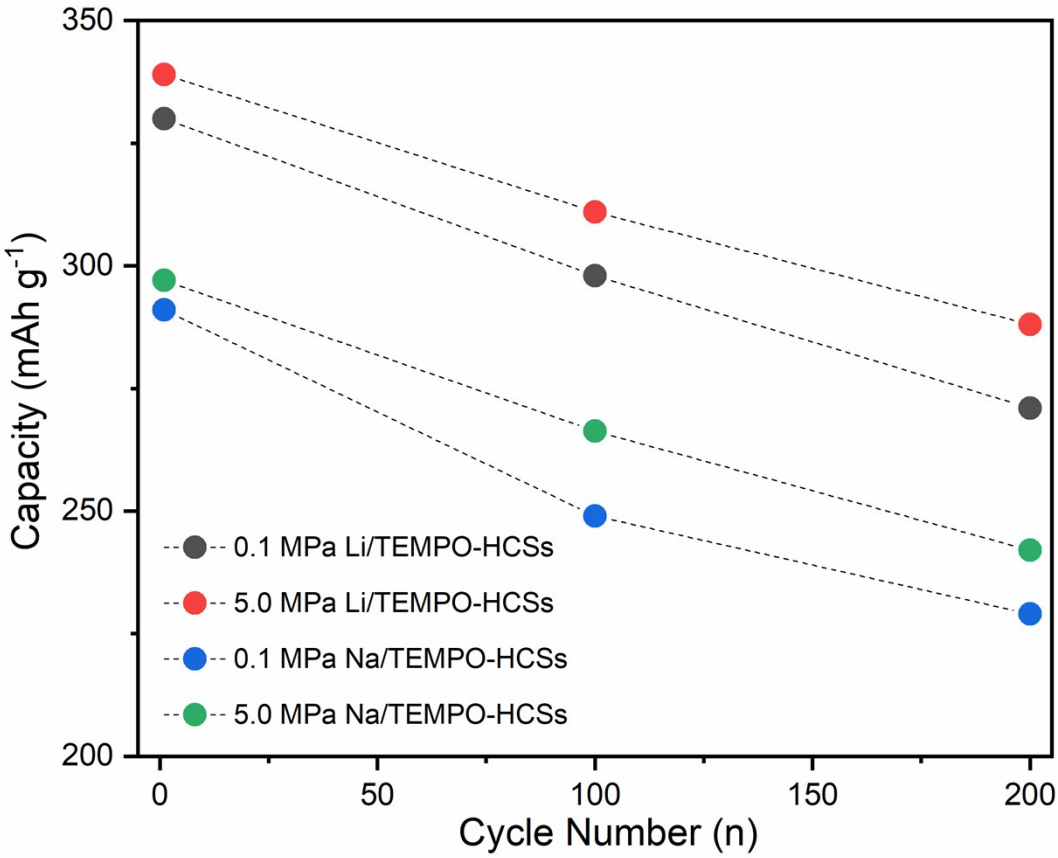
Supplementary Fig. S18 The Cycling profiles and columbic efficiency of Na/TEMPO-HCSs at 0.5 C in 5.0 MPa.



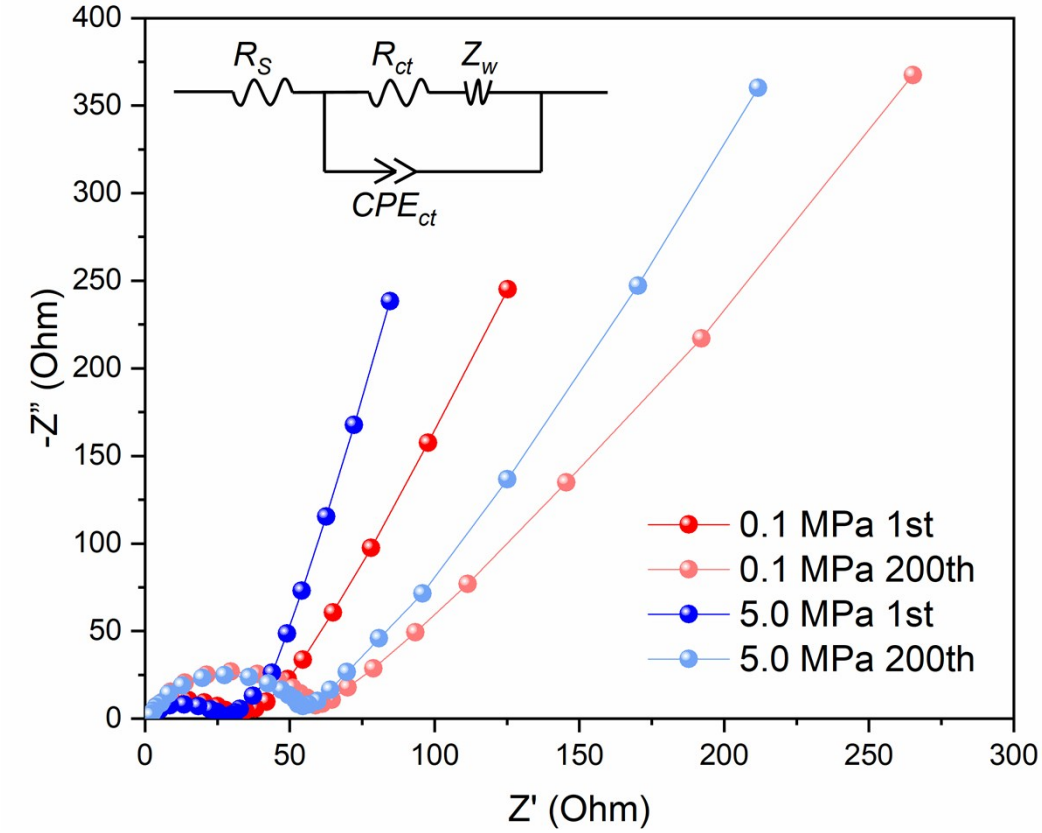
Supplementary Fig. S19 The Cycling profiles and columbic efficiency of Li/TEMPO-HCSs at 1 C in gradually changing pressure (0.1MPa-5MPa-0.1MPa, Rate of pressure change: 0.049MPa/h).



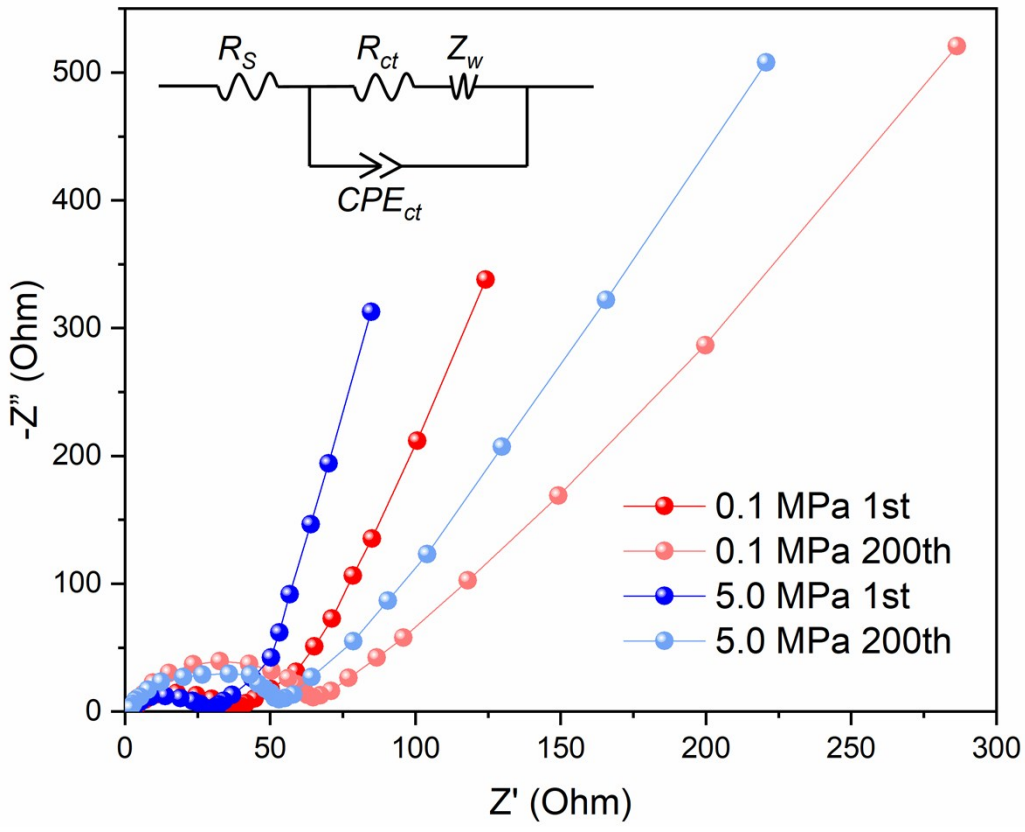
Supplementary Fig. S20 The Cycling profiles and columbic efficiency of Na/TEMPO-HCSs at 1 C in gradually changing pressure (0.1MPa-5MPa-0.1MPa, Rate of pressure change: 0.049MPa/h).



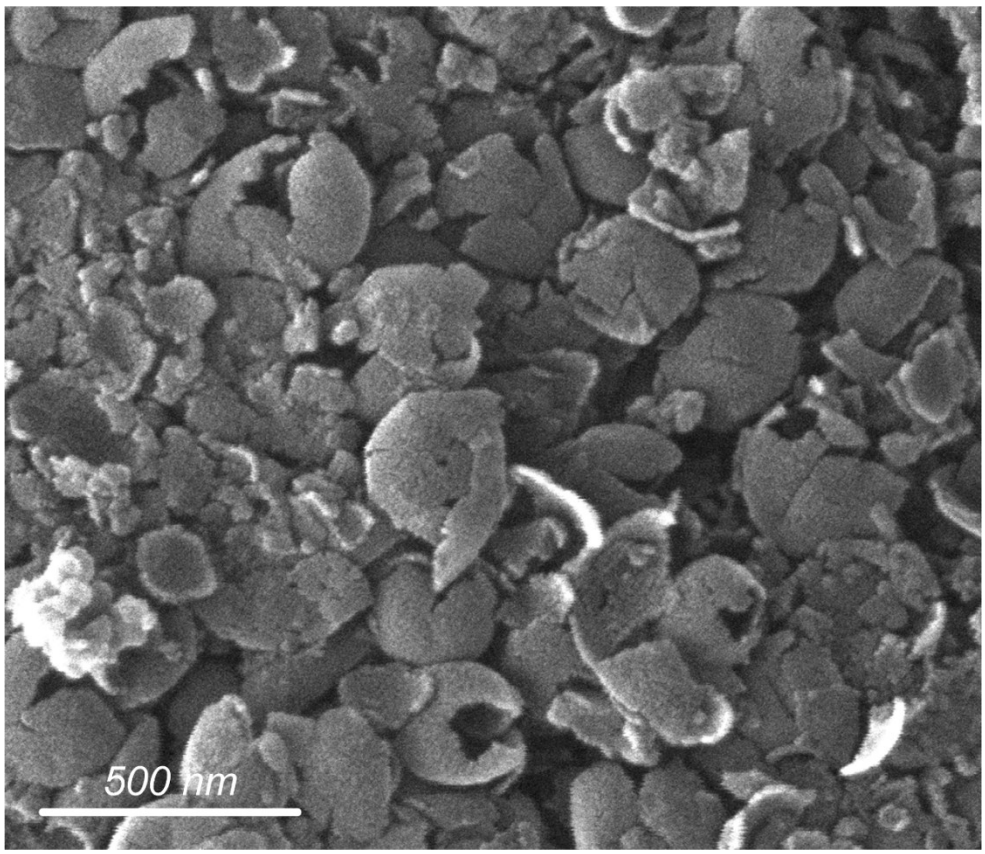
Supplementary Fig. S21 The comparison of cycling performance of Li/TEMPO-HCSs and Na/TEMPO-HCSs at 0.5 C in 50 atm.



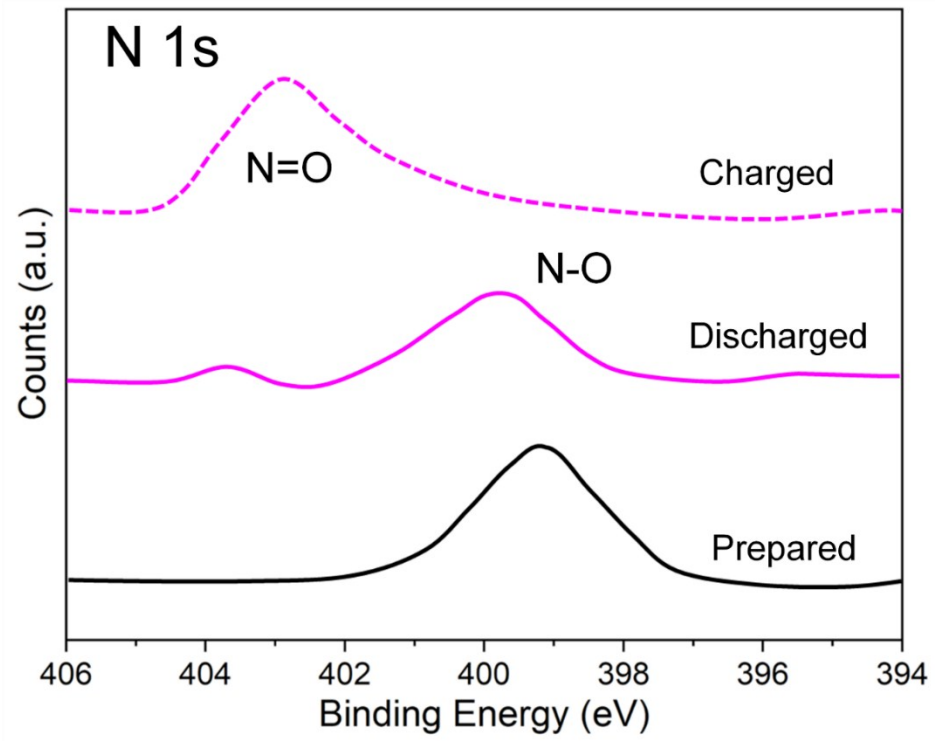
Supplementary Fig. S22 The electrochemical impedance spectroscopy (EIS) results of Li/TEMPO-HCSs at initial and after 200th cycle in different pressure.



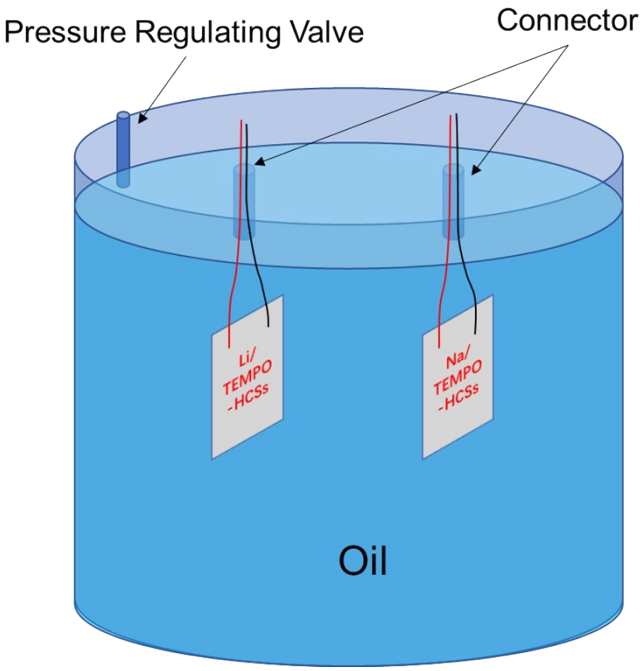
Supplementary Fig. S23 The electrochemical impedance spectroscopy (EIS) results of Na/TEMPO-HCSs at initial and after 200th cycle in different pressure.



Supplementary Fig. S24 SEM images of TEMPO–HCSs after 100 cycles



Supplementary Fig. S25 X-ray photoelectron spectroscopy (XPS) spectra in the N 1s region of TEMPO–HCSs (prepared, charged, and discharged).



Supplementary Fig. S26 The test device and details under different pressure of Li/TEMPO-HCSs and Na/TEMPO-HCSs.

Place Li/TEMPO-HCSs and Na/TEMPO-HCSs in a pressure tank filled with dielectric oil, and lead the wire through the interface to test the electrochemical performance of Li/TEMPO-HCSs and Na/TEMPO-HCSs. The pressure in the pressure tank is changed by the pressure regulating device to achieve the test of the electrochemical performance of Li/TEMPO-HCSs and Na/TEMPO-HCSs under different pressures.

References

1 Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.
2 L. Yongye, L. Yanguang, W. Hailiang, Z. Jigang, W. Jian, R. Tom and D. Hongjie, *Nat. Mater.*, 2011, **10**, 780-786.
3 V. Etacheri, C. Wang, M. J. O'Connell, C. K. Chan and V. G. Pol, *J. Mater. Chem. A.*, 2015, **3**, 9861-9868.
4 J. Han, G. Xu, B. Ding, J. Pan, H. Dou and D. R. MacFarlane, *J. Mater. Chem. A.*, 2014, **2**, 5352-5357.
5 R. Liu, S. M. Mahurin, C. Li, R. R. Unocic, J. C. Idrobo, H. Gao, S. J. Pennycook and S. Dai, *Angew. Chem. Int. Ed.*, 2011, **50**, 6799-6802.
6 D. Yan, Y. Li, D. Jing, M. Lang and X. Huang, *J. Polym. Sci. Pol. Chem.*, 2011, **49**, 4747-4755.
7 Z. Du, W. Ai, L. Xie and W. Huang, *J. Mater. Chem. A.*, 2014, **2**, 9164-9168.