Supplementary Information

Nitrogen-Doped Graphene Oxide: Toward Effective Removing Boron Ions from Sea Water

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Supplementary Tables and Figures:

Figure S1 the solution photos of brown GO (a) and dark brown N-GO-60 (b)

Table S1 the atomic ratio of N/C and O/C of GO, N-GO-x samples calculated from XPS results

Samples	GO	N-GO-RM	N-GO-40	N-GO-60	N-GO-80	N-GO-100	N-GO-140
N/C	0	0.035	0.043	0.062	0.073	0.077	0.093
O/C	0.39	0.038	0.034	0.335	0.301	0.249	0.129

Table S2 the boron absorption capacity and the corresponding removal efficiency (%) of N-GO at various temperatures during hydrothermal treatment

N-GO-x (x=hydrothermal temperature)	Absorption Capacity(mg/g)	Removal Efficiency (%)
GO	0.28	2.29
N-GO-RT	4.37	34.96
N-GO-40	4.81	38.48
N-GO-60	6.55	52.43
N-GO-80	6.21	48.89
N-GO-100	3.97	31.76
N-GO-140	0.47	3.74

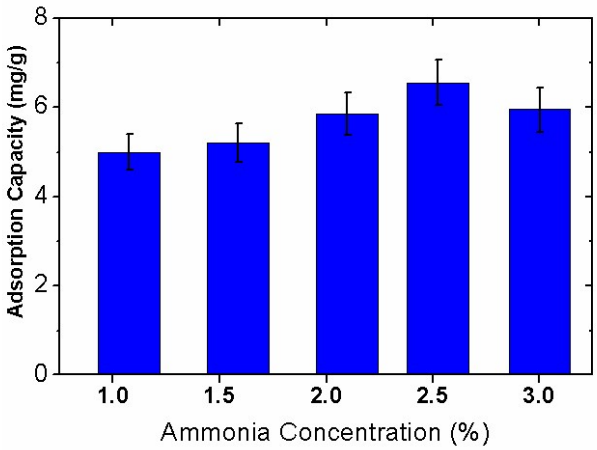

Figure S2 the effect from the various ammonia concentrations during hydrothermal treatment

Table S3 the boron absorption capacity and the corresponding removal efficiency (%) of N-GO at various ammonia concentrations during hydrothermal treatment

Hydrothermal Ammonia Concentration (%)	**Absorption Capacity(mg/g)**	**Removal Efficiency (%)**
1.07	4.99	39.97
1.59	5.21	41.68
2.10	5.85	46.83
2.52	6.55	52.43
3.00	5.95	47.63

Table S4 the atomic ratio of N/C and B/C of GO+B, N-GOx+B samples calculated from XPS results

Samples	**GO-B**	**N-GO-RT+B**	**N-GO-40+B**	**N-GO-60+B**	**N-GO-80+B**	**N-GO-100+B**	**N-GO-140+B**	**Boric acid**
N/C	0	0.0285	0.0338	0.065	0.071	0.072	0.088	0
B/C	0	0.101	0.131	0.188	0.122	0.073	0.060	0

Table S5 the kinetics absorption of boron for 5ppm boron feed (25 ml boron feed solution with 5 ppm boron was mixed with 40 mg N-GO media)

5ppm Feed Boron		
Time (hour)	**Absorption Capacity (mg/g)**	**Removal Efficiency (%)**
0.08	1.29	41.20
1	2.25	72.00
6	2.70	86.51
16	2.84	90.80
24	2.85	91.27
40	2.85	91.12

48	2.84	91.00

Table S6 the kinetics absorption of boron for 5ppm boron feed (25 ml boron feed solution with 20 ppm boron was mixed with 40 mg N-GO media)

20 ppm Feed Boron		
Time (hour)	**Absorption Capacity (mg g^{-1})**	**Removal Efficiency (%)**
0.08	3.25	26
1	5.17	41.36
6	6.45	51.6
16	6.55	52.4
24	6.52	52.16
40	6.55	52.4
48	6.56	52.48

Table S7 the kinetics absorption of boron for 20 ppm boron feed (25 ml boron feed solution with 100 ppm boron was mixed with 40 mg N-GO media)

100 ppm Feed Boron		
Time (hour)	**Absorption Capacity (mg g^{-1})**	**Removal Efficiency (%)**
0.08	5.28	8.45
1	7.56	12.10
6	10.29	16.46
16	11.56	18.49
24	11.55	18.49
40	11.57	18.51
48	11.55	18.47

Table S8 ppb level boron product obtained using 25 ml, 5 ppm feed with 110 mg N-GO-60

Feed Boron Concentration (ppm)	Product boron concentration (ppm)	Boron Rejection (%)
5	0.0630	98.74

Table S9 the effect from pH value on absorption capacity and the corresponding rejection, (25 ml boron feed solution with 20ppm boron was mixed with 40 mg N-GO media)

pH	**Absorption Capacity (mg g^{-1})**	**Removal Efficiency (%)**
2.01	5.25	41.97
4.80	5.98	47.80
8.57	6.55	52.40
10.53	5.99	47.92
13.01	5.70	45.61

Table S10 the Langmuir isotherm model (25 ml boron feed solution was mixed with 40 mg N-GO media)

C_e (ppm)	q_e (mg g^{-1})
0.45	2.84
9.52	6.55
36.06	8.71
81.49	11.57
681	43.11
922	49.02
2350	52.23
2916	53.36

Table S11 the effect from other ions (25 ml boron feed solution with 5 ppm boron was mixed with 40 mg N-GO media)

Samples	**Absorption Capacity (mg g^{-1})**	**Removal Efficiency (%)**
DI water	2.84	91.00
Simulated seawater	2.51	80.32
Real Seawater	2.42	77.44

Table S12 the regeneration of N-GO-60 using acid (25 ml boron feed solution with 20ppm boron was mixed with 40 mg N-GO media)

Cycles	**Absorption Capacity (mg g^{-1})**	**Removal Efficiency (%)**
1	6.55	52.40
2	5.63	45.04
3	5.32	42.56
4	5.18	41.44

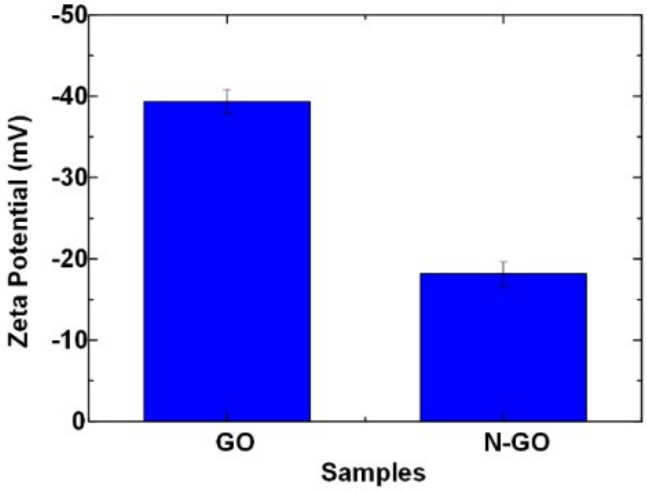

Figure S3. Comparison of zeta potential for GO and N-GO

First-principles calculations of the bonding energy: First-principles calculations are carried out by using the Vienna ab-initio simulation package (VASP), based on the density functional theory (DFT). The exchange-correlation functional is treated by using Perdew-Burke-Ernzerhof generalized gradient approximation. The cutoff for plane-wave expansion is set to be 400 eV. The atomic configuration positions and lattice constant were fully relaxed using conjugate gradient method. The convergence criteria for energy and force were set to be 10-6 eV and 0.01 eV/A, respectively. The Brillouin zone integrations have been carried out on a Γ -centered k-mesh. Monkhorst-Pack k-point meshes with sizes of 5 × 5 × 5 for geometry optimization. The bonding energy is defined as: $E_b = E_p - E_r$, where E_b , E_p and E_r are the bonding energy, the total energy of product compounds, and the total energy of product compounds, respectively. The Figure S1 below shows the two reactions. The calculated E_b corresponds to GO and N-GO reactions are equal to -1.87 and -2.67 eV respectively. This negative value of E_b, which indicates the feasibility of both reactions, implies the huge difference in adsorption capacities.

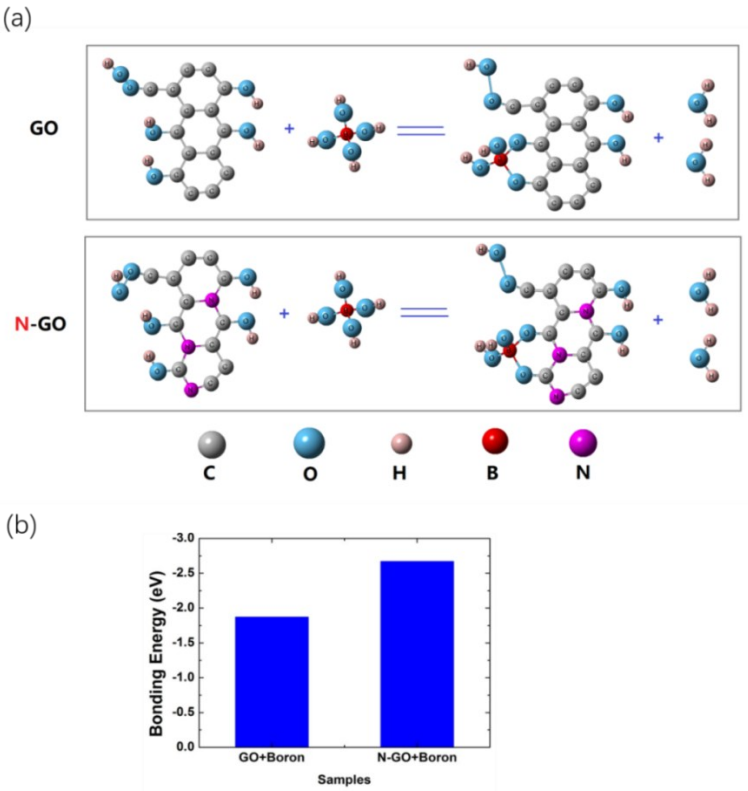

Figure S4 (a) Two reaction process and (b) the bonding energy between GO and boron species, as well as N-GO and boron species.