Supporting Information

Root exudates as natural ligands that alter the property of graphene oxide and environmental implications thereof

Junjie Du[a], Li Mu[b], Shaohu Ouyang[a], Chaoxiu Ren[a], Yingda Du[a], Xiangang Hu*[a] and Qixing Zhou*[a]

[a]Key Laboratory of Pollution Processes and Environmental Criteria (Ministry of Education), Tianjin Key Laboratory of Environmental Remediation and Pollution Control, College of Environmental Science and Engineering, Nankai University, Tianjin 300071, China.

[b]Institute of Agro-environmental Protection, Ministry of Agriculture, Tianjin 300191, China.

Correspondence atuhors:

* E-mail: huxiangang@nankai.edu.cn (X.H); zhouqx@nankai.edu.cn (Q.Z),

Phone: +86-022-23507800; fax: +86-022-66229562;

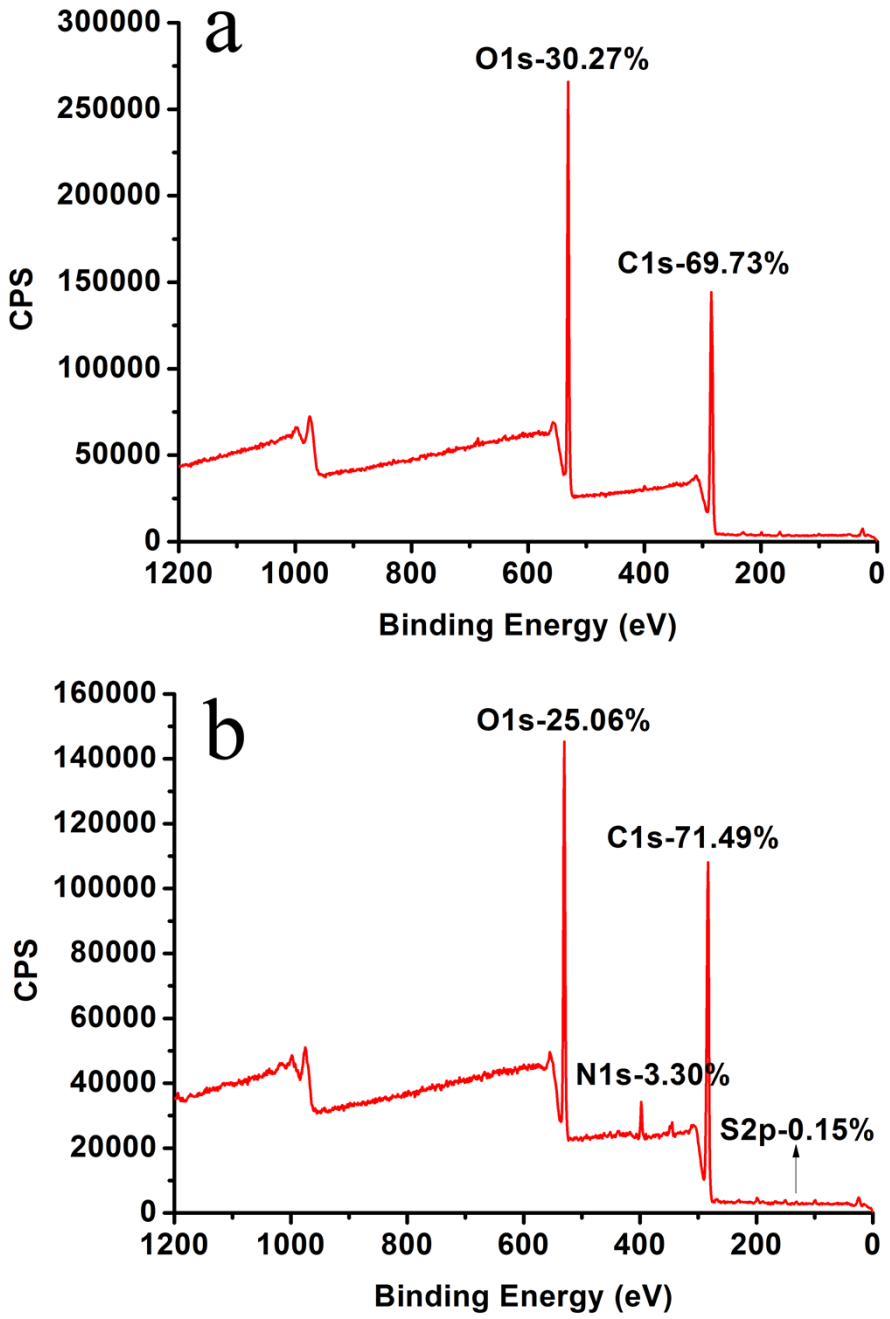

Figure S1. X-ray photoelectron spectra (XPS) of PGO and LGO: full spectrum of PGO (a) and full spectrum of LGO (b).

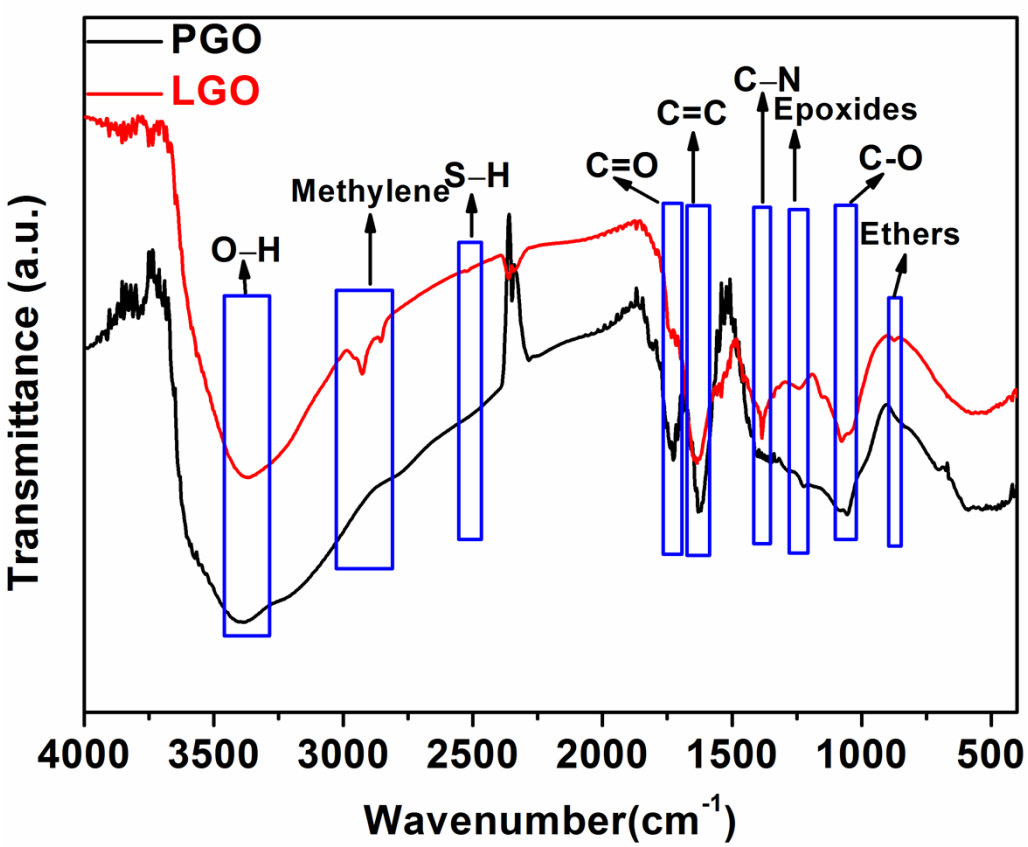

Figure S2. Fourier transform infrared spectroscopy (FTIR) spectra of PGO (pristine graphene oxide) and LGO (root exudates as ligand-graphene oxide complexes).

Table S1. Rice root exudates in the control without PGO exposure

Number	Name	Relative abundance[a]
1	Cyclohexanol	113002 ± 3251
2	Glycerol	207376 ± 10775
3	1,2-Propanediol	6344 ± 169
4	1-Butanol	12662 ± 605
5	Phenol	19692 ± 157
6	2-Butene-1,4-diol	23810 ± 1238
7	Methylbutanoic acid	19795 ± 675
8	Acetic acid	41467 ± 2126
9	Gluconic acid	4139 ± 313
10	Hexadecanoic acid	291474 ± 10537
11	Octadecanoic acid	313936 ± 6923
12	Benzenepropanoic acid	26716 ± 1062
13	Dodecanoic acid	1049 ± 64
14	tetradecanoic acid	71505 ± 2454
15	L-(+)-Lactic acid	17753 ± 726
16	Acetate	2993 ± 89
17	Xylose	1239 ± 28
18	1-Undecene	118451 ± 5444
19	Cyclohexen	4098 ± 86
20	Nonene	4160 ± 82
21	Propene	2345 ± 141
22	Hexanal	4680 ± 271
23	Benzaldehyde	18111 ± 343
24	Phenylpropane	6714 ± 286
25	Alkane (C2, C3, C5, C8, C10, C12, C13,C15, C16,C18)	345187 ± 11450

PGO, pristine graphene oxide.

[a] The errors are represented by standard errors (n = 3).

Table S2. Rice root exudates in the aqueous phase of PGO exposure group

Number	Name	Relative abundance[a]
1	Cyclohexanol	185344 ± 11034
2	Glycerol	240874 ± 4642
3	1,2-Propanediol	12974 ± 1057
4	1-Butanol	28568 ± 853
5	Phenol	10726 ± 513
6	2-Butene-1,4-diol	18087 ± 667
7	Isoborneol	5623 ± 253
8	Isobutyl alcohol	3032 ± 167
9	Geraniol	12834 ± 431
10	Geranylgeraniol	9809 ± 517
11	Oleyl alcohol	4811 ± 537
12	Ethanol	2287 ± 123
13	2-Octanol	9706 ± 162
14	Ethanethiol	22256 ± 1206
15	Methylbutanoic acid	23367 ± 742
16	Acetic acid	151031 ± 5379
17	Gluconic acid	19947 ± 1193
18	Hexadecanoic acid	264882 ± 6745
19	Octadecanoic acid	289647 ± 5612
20	Benzenepropanoic acid	52321 ± 1124
21	Dodecanoic acid	5360 ± 321
22	Tetradecanoic acid	71505 ± 2375
23	Octadecenoic acid	4403 ± 130
24	Oxiranecarboxylic acid	3336 ± 76
25	17-Octadecynoic acid	17463 ± 141
26	3-Cyclopentenecarboxylic acid	3641 ± 73
27	Octanoic acid	2332 ± 69
28	Pentanoic acid	4845 ± 120
29	Propanoic acid	3089 ± 79
30	Butanoic acid	1023 ± 83
31	Butanedioic acid	15155 ± 654
32	Cyclopropane-1-carboxylic acid	8357 ± 165
33	Benzenebutanoic acid	14696 ± 890
34	Ethanimidic acid	70222 ± 3587
35	Carbonodithioic O,S-acid	203914 ± 7342
36	Butyramide	50639 ± 2349
37	Alanine	6383 ± 532
38	Xylose	3573 ± 268
39	1-Undecene	101669 ± 863
40	Cyclohexen	4098 ± 432
41	Nonene	2285 ± 159
42	Hexanal	5586 ± 321

43	Nonanal	1427 ± 83
	Benzaldehyde	16816 ± 843
45	Benzenesulfonic acid	8512 ± 456
46	Phenylpropane	28007 ± 1403
47	Alkane (C2, C3, C5, C8, C10, C12, C13,C15, C16,C18)	80141 ± 8756

PGO, pristine graphene oxide.

[a] The errors are represented by standard errors (n = 3).

Table S3. Rice root exudates in the adsorption phase (LGO) of PGO exposure group

Number	Name	Relative abundance[a]
1	Glycerol	384050 ± 7296
2	Phenol	109727 ± 5596
3	Ethanethiol	22256 ± 178
4	Bisphenol	49636 ± 1346
5	Thymol	1600696 ± 85836
6	D-Mannitol	473459 ± 19411
7	Geraniol	16994 ± 611
8	Hexadecanoic acid	2415764 ± 125619
9	Octadecanoic acid	211500 ± 6345
10	2-Monostearin	151424 ± 4537
11	Azelaic acid	110322 ± 3971
12	Benzenepropanoic acid	25315 ± 699
13	Phthalic acid	37753 ± 1515
14	Benzenebutanoic acid	51395 ± 2021
15	1,4-Benzenedicarboxylic acid	140847 ± 3239
16	Salicylic acid	365692 ± 13164
17	Ethanimidic acid	70222 ± 1631
18	4-Pentenoic acid	20444 ± 1034
19	Myristic acid	55058 ± 1385
20	Carbonodithioic O,S-acid	203914 ± 10191
21	Ethanedioic acid	154734 ± 2321
22	Butanedioic acid	86591 ± 1771
23	Butylated hydroxytoluene	125458 ± 6398
24	Undecene	22543 ± 202
25	Coronene	2455149 ± 61471
26	Butyramide	50639 ± 208
27	Propiophenone	25572 ± 251
28	Benzaldehyde	25081 ± 332
29	9-Acetylphenanthrene	78996 ± 157
30	Cyclohexene	1823776 ± 9299
31	Pentacosane	33140 ± 1230

PGO, pristine graphene oxide; LGO, root exudates as ligands-graphene oxide.

[a] The errors are represented by standard errors (n = 3).