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How are oxygen budgets influenced by dissolved iron and growth of oxygenic phototrophs in an iron-rich spring system? Initial results from the Espan Spring in Fürth, Germany

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Supporting information

Table S1: PhreeqC input data

Input (cold)*	**E1a**	**E1b**	**E2**	**E3**	**E3.1**	**E4**	**E4.1**	**E5**	**E5.1**	**E6**	**E6.1**	**E7**	**E8**	**E9**
pH	6.1	6.5	6.5	6.7	6.5	7.1	7.5	7.9	7.6	7.9	7.9	7.9	8.0	8.6
pe	4.6	4.3	4.2	4.1	3.6	3.3	2.9	2.8	2.7	2.8	3.3	4.1	5.2	7.0
density	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
temp	19.5	19.3	19.3	17.5	17.5	16.2	16.1	15.2	15.3	14.1	13.3	12.3	10.8	11.0
Na	2500	2500	2500	2500	2500	2500	2500	2400	2500	2500	2500	2400	92	23
Mg	166	163	165	165	165	164	164	164	166	166	165	162	18	14
Si	4.9	4.8	4.8	4.7	4.7	4.8	4.7	4.7	4.6	4.6	4.6	4.6	2.8.	2.7
K	200	200	200	200	200	200	200	200	200	200	200	200	11	5
Ca	1200	1200	1200	1200	1200	1200	1200	1200	1200	1200	1200	1100	91	60
Li	3.2	3.2	3.2	3.3	3.3	3.2	3.1	3.1	3.2	3.1	3.2	3.2	0.0	0.0
B	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.8	0.9	0.9	0.0	0.0
Cl	4400	4500	4500	4500	4500	4500	4500	4500	4500	4500	4500	4500	170	38
S(6)	2100	2200	2200	2200	2200	2200	2200	2200	2200	2200	2200	2200	92	30
Fe(II)	6.6	6.6	5.6	5.7	4.5	3.9	3.4	0.9	0.4	0.2	0.0	0.0	0.0	0.0
Alkal.**	820	828	796	790	810	804	808	804	816	760	770	760	195	160

Input (warm)*	**E1a**	**E1b**	**E2**	**E3**	**E3.1**	**E4**	**E4.1**	**E5**	**E5.1**	**E6**	**E6.1**	**E7**	**E8**	**E9**
pH	6.3	6.4	6.5	6.6	6.9	7.2	7.3	7.4	7.5	7.5	7.5	7.5	7.5	8.0
pe	5.4	5.0	5.1	5.2	4.8	5.0	5.0	5.8	6.5	6.6	6.9	4.1	5.2	7.0
density	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
temp	21.3	21.2	20.6	21.6	22.5	22.7	23.0	24.0	25.6	25.7	25.5	24.9	22.8	16.8
Na	2500	2500	2500	2500	2500	2500	2500	2500	2500	2500	2500	2500	170	90
Mg	180	180	170	170	170	180	170	170	170	180	170	170	33	10
Si	4.8	4.8	4.7	4.6	4.7	4.8	4.7	4.6	4.9	4.6	4.6	4.9	3.0	2.4
K	210	210	210	210	210	210	210	210	210	210	210	210	22	10
Ca	1200	1200	1200	1200	1200	1200	1200	1200	1200	1200	1200	1100	120	90
Li	3.2	3.2	3.2	3.2	3.2	3.2	3.2	3.2	3.2	3.2	3.2	3.2	3.2	0.0
B	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.0	0.0
Cl	4500	4400	4400	4400	4400	4400	4500	4500	4500	4500	4500	4500	290	110
S(6)	2200	2200	2100	2200	2200	2200	2200	2200	2200	2200	2200	2200	150	56
Fe(II)	6.9	6.7	5.6	4.0	2.9	1.5	0.7	0.1	0.0	0.0	0.0	0.0	0.0	0.0
Alkal.**	874	850	846	814	808	826	812	786	804	796	748	742	708	238

* units ppm
** Alkalinity as ppm $CaCO_3$

Table S2: PhreeqC output data

Phase (cold)	**SI***	**Log IAP****	**Log K (202 K,1 atm)**
E1a			
Ferrihydrite	0.13	5.02	4.89
Goethite	5.83	5.03	-0.80
Hematite	13.64	10.05	-3.58

Phase	**SI***	**Log IAP****	**Log K (202 K,1 atm)**
E1b			
Ferrihydrite	1.06	5.95	4.89
Goethite	6.74	5.95	-0.79
Hematite	15.47	11.90	-3.57
Siderite	0.34	-10.51	-10.85

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E2			
Ferrihydrite	1.01	5.90	4.89
Goethite	6.70	5.90	-0.79
Hematite	15.38	11.81	-3.57
Siderite	0.30	-10.56	-10.85

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E3			
Ferrihydrite	1.45	6.34	4.89
Goethite	7.07	6.35	-0.73
Hematite	16.12	12.69	-3.42
Siderite	0.47	-10.37	-10.84

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E3.1			
Ferrihydrite	0.33	5.22	4.89
Goethite	5.95	5.23	-0.73
Hematite	13.88	10.45	-3.42
Siderite	0.19	-10.65	-10.84

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E4			
Ferrihydrite	1.70	6.60	4.89
Goethite	7.28	6.60	-0.68
Hematite	16.52	13.20	-3.32
Siderite	0.68	-10.15	-10.83

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E4.1			
Ferrihydrite	2.20	7.09	4.89
Goethite	7.77	7.09	-0.67
Hematite	17.50	14.19	-3.31
Siderite	0.97	-9.86	-10.83

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E5			
Ferrihydrite	2.81	7.70	4.89
Goethite	8.34	7.70	-0.64
Hematite	18.64	15.40	-3.24
Siderite	0.68	-10.14	-10.83

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E5.1			
Ferrihydrite	1.47	6.36	4.89
Goethite	7.01	6.36	-0.64
Hematite	15.98	12.73	-3.25
Siderite	0.16	-10.67	-10.83

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E6			
Ferrihydrite	2.02	6.91	4.89
Goethite	7.51	6.91	-0.60
Hematite	16.98	13.83	-3.15
Siderite	0.06	-10.76	-10.82

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E6.1* **			
Ferrihydrite	1.35	6.24	4.89
Goethite	6.81	6.24	-0.57
Hematite	15.57	12.48	-3.08

Phase (warm)	SI*	Log IAP**	Log K (202 K,1 atm)
E1a			

Ferrihydrite	1.67	6.56	4.89
Goethite	7.43	6.57	-0.87
Hematite	1686	13.13	-3.72

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E1b			
Ferrihydrite	1.57	6.46	4.89
Goethite	7.33	6.47	-0.86
Hematite	16.65	12.93	-3.72
Siderite	0.33	-10.53	-10.87

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E2			
Ferrihydrite	1.87	6.76	4.89
Goethite	7.61	6.77	-0.84
Hematite	17.21	13.54	-3.67
Siderite	0.34	-10.52	-10.86

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E3			
Ferrihydrite	2.16	7.05	4.89
Goethite	7.93	7.05	-0.88
Hematite	17.85	14.10	-3.75
Siderite	0.30	-10.57	-10.87

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E3.1			
Ferrihydrite	2.55	7.44	4.89
Goethite	8.35	7.44	-0.91
Hematite	18.70	14.88	-3.82
Siderite	0.47	-10.40	-10.87

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E4			
Ferrihydrite	2.99	7.88	4.89
Goethite	8.80	7.88	-0.92
Hematite	19.60	15.77	-3.83
Siderite	0.52	-10.36	-10.88

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E4.1			
Ferrihydrite	3.21	8.10	4.89
Goethite	9.03	8.10	-0.93
Hematite	20.06	16.20	-3.86
Siderite	0.13	-10.75	-10.88

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E5			
Ferrihydrite	3.26	8.15	4.89
Goethite	9.12	8.15	-0.96
Hematite	20.24	16.31	-3.93
Siderite	-	-	-

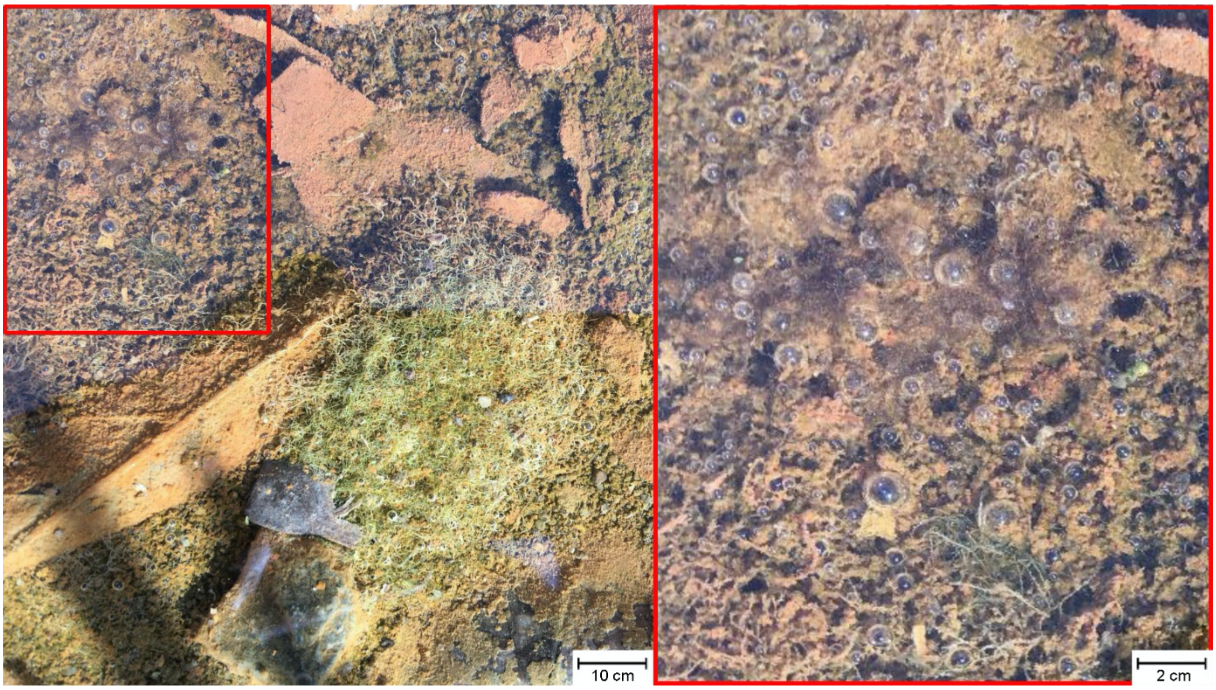
Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E5.1			
Ferrihydrite	-	-	-
Goethite	-	-	-
Hematite	-	-	-
Siderite	-	-	-

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
E6			
Ferrihydrite	-	-	-
Goethite	-	-	-

Hematite	-	-	-
Siderite	-	-	-
Phase	**SI***	**Log IAP****	**Log K (202 K,1 atm)**
E6.1* **			
Ferrihydrite	-	-	-
Goethite	-	-	-
Hematite	-	-	-
Phase	**SI***	**Log IAP****	**Log K (202 K,1 atm)**
E7* **			
Ferrihydrite	-	-	-
Goethite	-	-	-
Hematite	-	-	-
Phase	**SI***	**Log IAP****	**Log K (202 K,1 atm)**
E8* **			
Ferrihydrite	-	-	-
Goethite	-	-	-
Hematite	-	-	-
Phase	**SI***	**Log IAP****	**Log K (202 K,1 atm)**
E9* **			
Ferrihydrite	-	-	-
Goethite	-	-	-
Hematite	-	-	-

* Saturation index = log10(fugacity)
** Ion activity product
*** Last sampling point with Fe(II)

Supplement Figure S1 At sampling point E4.1, Lyngby asp. dominated cyanobacterial mats and generated (presumed) oxygen bubbles via photosynthesis. The red box on the right is an enlargement of the red section on the left.



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Supplement Figure S2. CLSM images of the bio mat sample E2 from inside the piping. Shown from left to right are a superimposed image (Overlay) of Chl a (Chl a), Chl a plus PBP (Chl a plus PBP) fluorescence and laser transmission (L. Trans.). Note that the images "Overlay" and "L. Trans." are colourless because no photosynthetic organisms existed in the area where these specific samples were taken due to spring plumbing. The two middle images show some small green and red dots that are probably artefacts. These were likely created by the very high laser intensity that was necessary to create these images.