A. Supplementary tables

Table S1. A summary of reads information and microbial classification at different taxonomic levels.

Table S2. Pearson's correlations between the abundance of diazotrophic genera and the nitrogen fixation rate (NFR).

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B. Supplementary figures

Fig. S1. The location of the sampling habitats at the Qi'ao Island, Guangdong Province, China.

Fig. S2. Relationships between the depth of mangrove sediments and the NFR (**a**), water content (**b**), salinity (**c**), Shannon index (**d**) and Chao1 index (**e**). NFR was represented as acetylene reduction (nmol g^{-1} h^{-1}) in this research. Black lines and grey shaded areas represent linear regressions and 95% confidence intervals, respectively. R^2 was obtained by linear regression analysis and *p* was obtained by Pearson's correlation analysis.

Fig. S3. The in-depth profile of physicochemical properties. The concentration of NH_4^+ (**a**), NO_2^- (**b**), NO_3^- (**c**), pH (**d**), water content (**e**), salinity (**f**), total Fe (**g**), available Fe (**h**) and Fe^{3+} (**i**) across 10 depths of mangrove sediments. Boxplots depict the 25-75% quantile range of the selected measurements, with the centerline depicting the median (50% quantile). Whiskers show the minimum and maximum values.

Fig. S4. Bray-Curtis distance-based hierarchical clustering of diazotrophic communities across 10 depths of mangrove sediments. The color gradient represents sediment depth.

A. Supplementary tables

Table S1. A summary of reads information and microbial classification at different taxonomical levels.

Samples	Reads	OTUs	Phylum	Class	Order	Family	Genus	Species
S1-0-10cm	86195	718	5	9	22	34	49	90
S2-0-10cm	70481	758	5	10	22	34	52	94
S3-0-10cm	80416	772	6	10	22	35	51	94
S4-10-20cm	66846	820	5	10	24	37	56	101
S5-10-20cm	100501	789	5	10	23	36	54	96
S6-10-20cm	81996	736	6	11	23	36	54	98
S7-20-30cm	68499	779	6	10	21	35	52	97
S8-20-30cm	64514	787	5	10	22	36	53	97
S9-20-30cm	87197	776	5	10	23	37	56	98
S10-30-40cm	83713	783	5	10	23	37	54	96
S11-30-40cm	74631	690	3	8	21	31	46	85
S12-30-40cm	66249	805	5	10	24	38	53	94
S13-40-50cm	67937	854	6	11	24	37	55	100
S14-40-50cm	73389	747	4	8	21	34	52	91
S15-40-50cm	91327	843	5	10	23	37	54	97
S16-50-60cm	73672	863	6	11	25	39	56	99
S17-50-60cm	54512	748	6	11	24	37	52	92
S18-50-60cm	58440	816	4	9	23	37	55	96
S19-60-70cm	89734	789	6	11	23	37	54	96
S20-60-70cm	86355	625	6	11	25	37	53	86
S21-60-70cm	74963	664	5	10	23	35	52	89
S22-70-80cm	74963	725	6	10	23	35	50	91

S23-70-80cm	104660	719	6	11	24	36	51	90
S24-70-80cm	100077	627	4	8	22	31	46	79
S25-80-90cm	54074	696	5	10	23	35	53	92
S26-80-90cm	65338	758	5	10	23	35	50	92
S27-80-90cm	71914	579	6	11	24	36	48	77
S28-90-100cm	57216	777	6	11	25	38	55	96
S29-90-100cm	60295	654	5	10	23	36	50	86
S30-90-100cm	60282	761	5	11	24	37	55	91
Total	2253352	974	6	11	25	39	58	103

Table S2. Pearson's correlations between the abundance of diazotrophic genera and the nitrogen fixation rate (NFR).

Genus	*Bradyrhizobium*	*Geobacter*	*Azotobacter*	*Halorhodospira*	*unidentified*	*Desulfovibrio*
r-value	-0.326	-0.277	0.693*	-0.507	0.540	-0.750*
p-value	0.358	0.439	0.026	0.135	0.107	0.012
Genus	*Dechloromonas*	*Agrobacterium*	*Anaeromyxobacter*	*Marichromatium*	*Pelobacter*	*Desulfobulbus*
r-value	0.003	0.853**	-0.726*	-0.830**	0.430	0.161
p-value	0.993	0.002	0.017	0.003	0.215	0.657
Genus	*Pseudomonas*	*Rubrivivax*	*Azohydromonas*	*Pseudodesulfovibrio*	*Methylobacterium*	*Desulfatibacillum*
r-value	-0.756*	-0.711*	-0.216	-0.433	-0.677*	0.478
p-value	0.010	0.021	0.549	0.211	0.031	0.162
Genus	*Sinorhizobium*	*Azoarcus*	*Zoogloea*	*Pelomonas*	*Ideonella*	*Azospirillum*
r-value	-0.186	-0.464	0.563	-0.581	0.444	-0.674*
p-value	0.607	0.177	0.090	0.078	0.198	0.033
Genus	*Dehalococcoides*	*Geoalkalibacter*	*Ectothiorhodospira*	*Methylomonas*	*Desulfuromonas*	*Dickeya*
r-value	0.122	-0.426	-0.282	-0.638*	0.450	-0.648*
p-value	0.738	0.219	0.431	0.047	0.192	0.043
Genus	*Sideroxydans*	*Thiocapsa*	*Desulfarculus*	*Sulfuricurvum*	*Chlorobaculum*	*Azomonas*
r-value	-0.533	-0.729*	-0.567	0.163	0.323	-0.345
p-value	0.112	0.017	0.087	0.652	0.362	0.329
Genus	*Methylocystis*	*Klebsiella*	*Methanoregula*	*Azorhizobium*	*Rhodobacter*	*Xanthobacter*
r-value	-0.772**	0.325	0.246	-0.168	-0.207	-0.484
p-value	0.009	0.360	0.493	0.642	0.567	0.156
Genus	*Pelosinus*	*Allochromatium*	*Heliobacterium*	*Desulfurivibrio*	*Methanothrix*	*Nitratireductor*
r-value	-0.618	0.408	-0.289	-0.021	0.148	-0.116

p-value	0.057	0.241	0.418	0.953	0.683	0.749
Genus	*Methanocella*	*Thioalkalispira*	*Magnetospirillum*	*Azospira*	*Thiorhodococcus*	*Vibrio*
r-value	-0.186	-0.373	-0.546	0.538	-0.213	0.096
p-value	0.607	0.288	0.103	0.108	0.554	0.193
Genus	*Leptothrix*	*Candidatus_Accumulibacter*	*Paraburkholderia*	*Rhodopseudomonas*	*Methylococcus*	
r-value	-0.429	-0.101	-0.383	-0.482	-0.620	
p-value	0.216	0.780	0.274	0.158	0.056	

Note: *: $p < 0.05$ means a significant correlation, **: $p < 0.01$ is very significant.

Table S3. Relative abundances of diazotrophic communities at the genus level.

Genus	*Bradyrhizobium*	*Geobacter*	*Azotobacter*	*Halorhodospira*	*unidentified*	*Desulfovibrio*
Average relative abundance (%)	15.18 ± 5.51	14.74 ± 4.87	11.92 ± 13.9	11.12 ± 4.46	8.59 ±5.20	5.19 ± 3.51
Genus	*Dechloromonas*	*Agrobacterium*	*Anaeromyxobacter*	*Marichromatium*	*Pelobacter*	*Desulfobulbus*
Average relative abundance (%)	3.51 ± 3.87	3.28 ± 5.19	2.88 ± 3.12	2.81 ± 1.21	2.68 ± 1.67	2.64 ± 1.69
Genus	*Pseudomonas*	*Rubrivivax*	*Azohydromonas*	*Pseudodesulfovibrio*	*Methylobacterium*	*Desulfatibacillum*
Average relative abundance (%)	1.70 ± 1.09	1.64 ± 1.39	1.38 ± 2.43	1.32 ± 0.86	1.01 ± 0.81	0.91 ± 2.30
Genus	*Sinorhizobium*	*Azoarcus*	*Zoogloea*	*Pelomonas*	*Ideonella*	*Azospirillum*
Average relative abundance (%)	0.70 ± 0.91	0.58 ± 0.71	0.52 ± 0.50	0.51 ± 0.94	0.48 ± 0.38	0.45 ± 0.44
Genus	*Dehalococcoides*	*Geoalkalibacter*	*Ectothiorhodospira*	*Methylomonas*	*Desulfuromonas*	*Dickeya*
Average relative abundance (%)	0.45 ± 1.32	0.44 ± 0.59	0.40 ± 0.33	0.33 ± 0.41	0.28 ± 0.70	0.25 ± 0.22
Genus	*Sideroxydans*	*Thiocapsa*	*Desulfarculus*	*Sulfuricurvum*	*Chlorobaculum*	*Azomonas*
Average relative abundance (%)	0.18 ± 0.23	0.18 ± 0.12	0.14 ± 0.12	0.14 ± 0.19	0.12 ± 0.39	0.12 ± 0.33
Genus	*Methylocystis*	*Klebsiella*	*Methanoregula*	*Azorhizobium*	*Rhodobacter*	*Xanthobacter*

Average relative abundance (%)	0.11 ± 0.11	0.09 ± 0.20	0.08 ± 0.27	0.08 ± 0.13	0.08 ± 0.06	0.08 ± 0.06
Genus	*Pelosinus*	*Allochromatium*	*Heliobacterium*	*Desulfurivibrio*	*Methanothrix*	*Nitratireductor*
Average relative abundance (%)	0.08 ± 0.09	0.07 ± 0.08	0.06 ± 0.09	0.6 ± 0.08	0.05 ± 0.05	0.05 ± 0.09
Genus	*Methanocella*	*Thioalkalispira*	*Magnetospirillum*	*Azospira*	*Thiorhodococcus*	*Vibrio*
Average relative abundance (%)	0.05 ± 0.06	0.05 ± 0.14	0.04 ± 0.05	0.03 ± 0.04	0.03 ± 0.05	0.03 ± 0.04
Genus	*Leptothrix*	*Candidatus_ Accumulibacter*	*Paraburkholderia*	*Rhodopseudomonas*	*Methylococcus*	
Average relative abundance (%)	0.02 ± 0.04	0.02 ± 0.05	0.02 ± 0.14	0.02 ± 0.03	0.02 ± 0.02	

Note: Data are shown as means ± SD.

Table S4. Mantel test for the correlations between diazotrophic community structure and sediment properties.

Correlation between diazotrophic community structure and:	Mantel r	*p*
Salinity	0.477**	**< 0.01**
pH	0.240**	**< 0.01**
Fe^{3+}	0.237**	**< 0.01**
Water content	0.209**	**< 0.01**
NH_4^+	0.192*	**< 0.05**
NO_3^-	0.075	≥ 0.05
NO_2^-	0.010	≥ 0.05
Total Fe	0.002	≥ 0.05
Available Fe	-0.06	≥ 0.05

Note: Bold value indicates $p < 0.05$. (*: $p < 0.05$; **: $p < 0.01$)

B. Supplementary figures

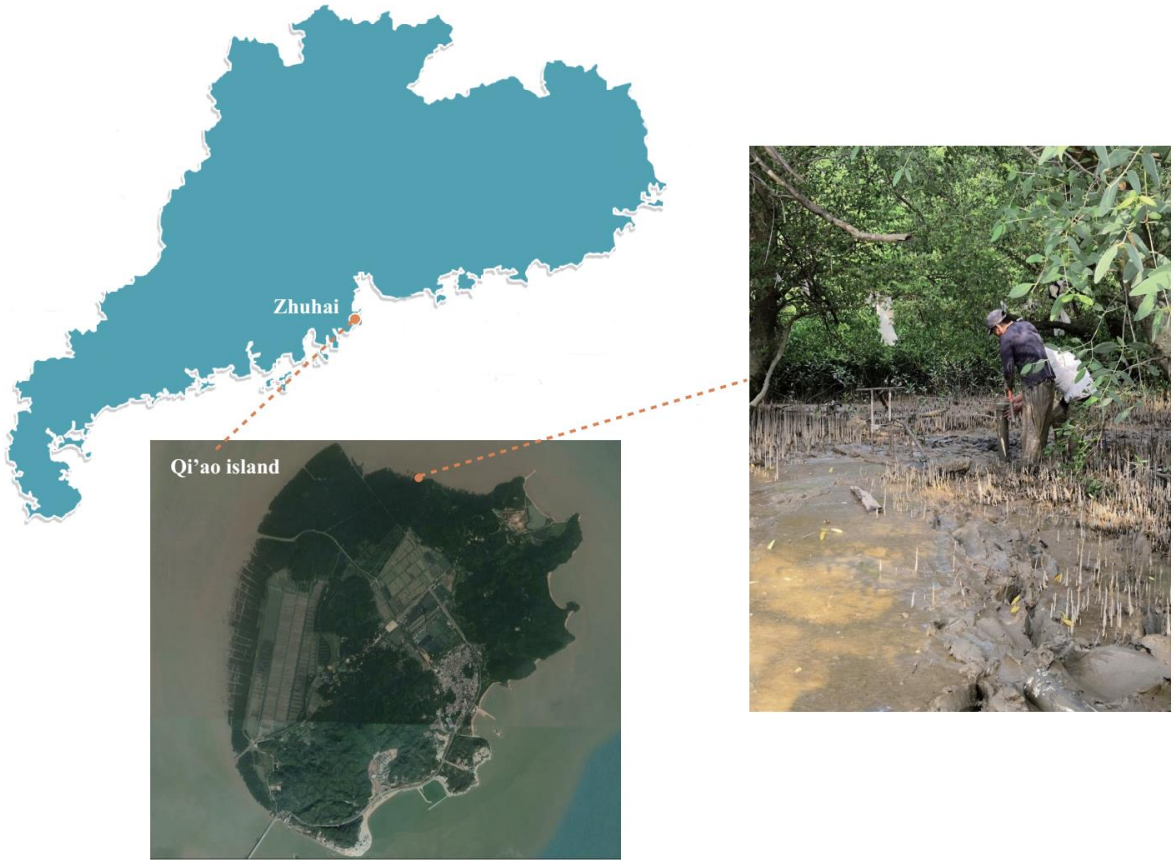
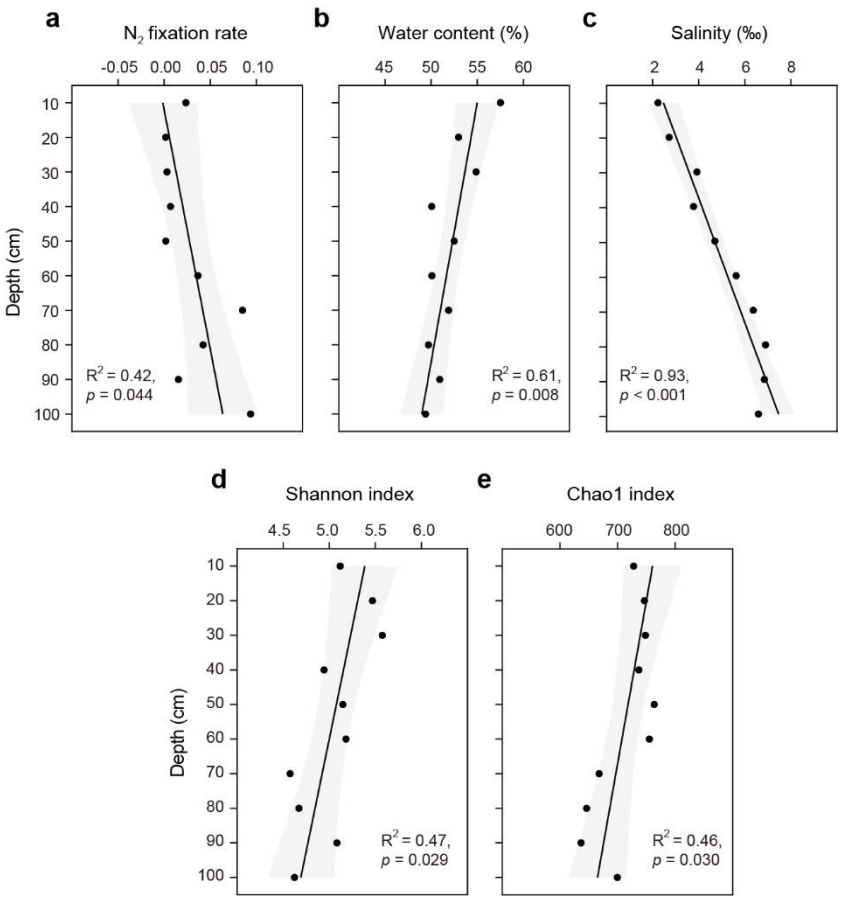


Fig. S1. The location of the sampling habitats at the Qi'ao Island, Guangdong Province, China.



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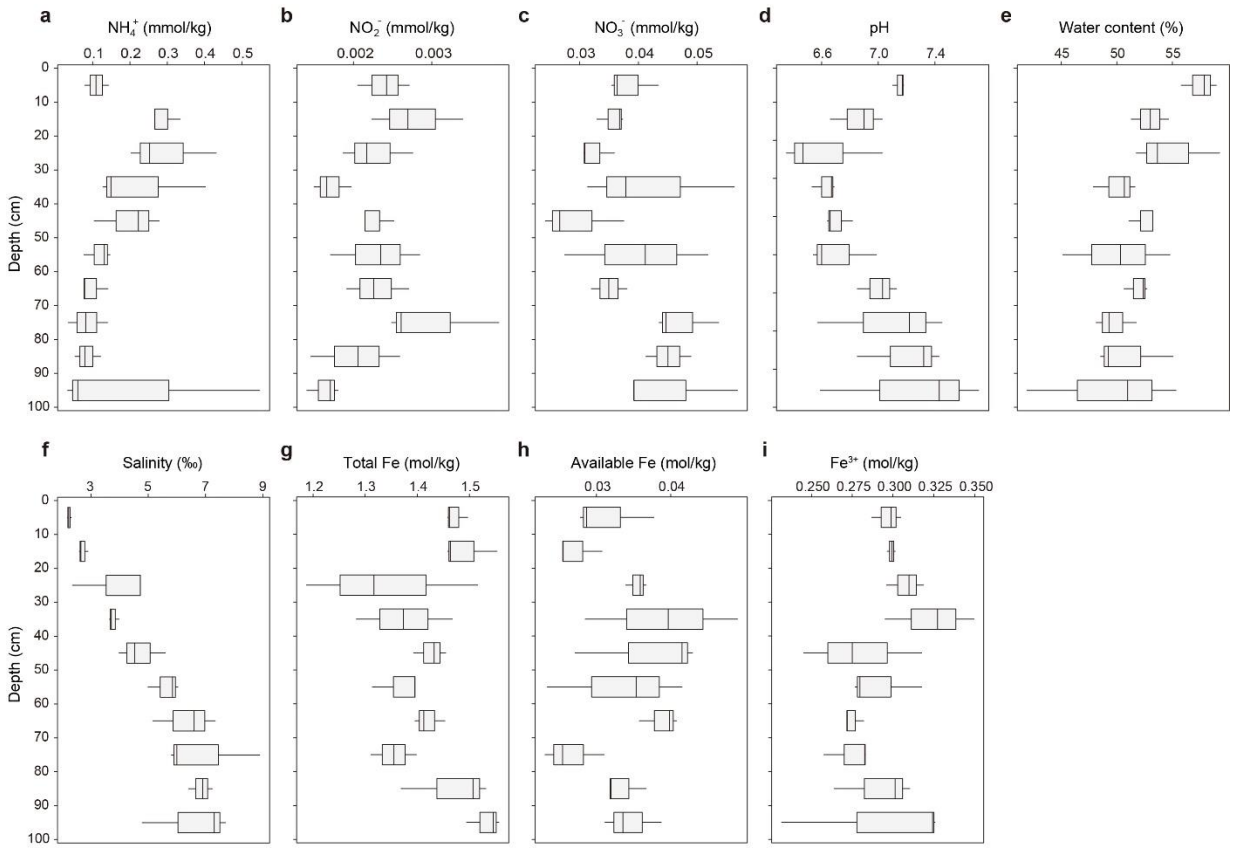

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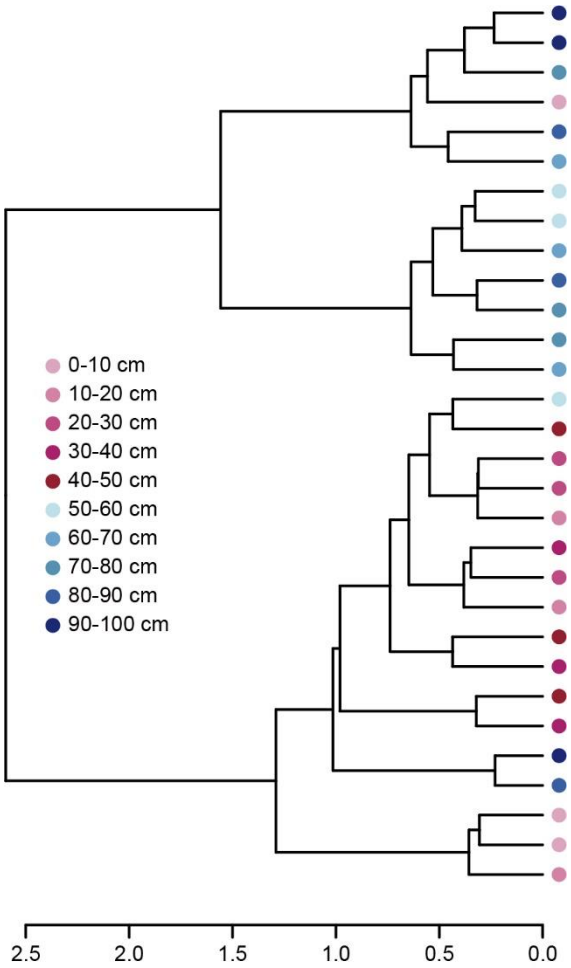

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