Table 1 The geometric structures of initial state, medium state and final state of oxygen dissociation on different carbon structures (unit: Å)

Structure		Initial state	Medium state	Final state
Fig. 1a	do-o	1.24	1.51	3.02
	average dc-o	3.31	1.48	1.45
Fig. 1b	dc-o	1.25	1.51	2.77
	average dc-o	3.31	1.48	1.45
	dc=o			1.29
Fig. 1c	do-o	1.37	1.51	2.75
	dc-o	1.48	1.56	1.46(average)
		2.32	1.45	
	dc=o			1.22
Fig. 1d	do-o	1.25	1.50	2.76
	average dc-o	3.51	1.47	
	average dc=o			1.23
Fig. 1e	do-o	1.33	1.51	2.40
	dc-o	1.51	1.44	1.32
		2.35	1.65	1.65
	dc=o			1.23
Fig. 1f	do-o	1.24	1.51	2.65
	average dc-o	3.58	1.45	
	average dc=o			1.22
Fig. 2a	do-o	1.24	1.50	2.87
	average dc-o	3.55	1.50	1.47
Fig. 2b	do-o	1.26	1.49	2.67
	average dc-o	3.31	1.51	1.45
	dc=o			1.30
Fig. 2c	do-o	1.26	1.49	2.65
	average dc-o	3.09	1.50	
	dc=o			1.31
Fig. 2d	do-o	1.24	1.49	2.80
	average dc-o	3.47	1.49	1.45

Table 2 The energy barriers and the adsorption energies of initial state, medium state and final state of oxygen dissociation on different carbon structures (unit: eV)

structure	Initial state	Medium state	Final state	$Barrier_1$	$Barrier_2$	$Barrier_{total}$
Fig. 1a	0.01	-0.92	0.27	1.61	1.43	1.61
Fig. 1b	0.04	-0.49	0.39	0.86	0.70	0.86
Fig. 1c	0.18	-0.11	1.97	0.35	0.42	0.42
Fig. 1d	0.11	0.64	2.70	0.69	-0.18	0.69
Fig. 1e	0.49	0.37	3.70	0.49	0.30	0.49
Fig. 1f	0.01	-0.44	1.18	1.28	1.24	1.28
Fig. 2a	0.03	-2.08	-1.53	2.62	2.71	2.71
Fig. 2b	0.14	-1.41	-0.95	1.73	1.87	1.87
Fig. 2c	0.19	0.30	1.56	0.19	0.02	0.19
Fig. 2d	0.12	-1.53	-1.11	1.71	2.34	2.34

The Fig. 1 and Fig. 2 are showed in the main text.