Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY

TABLE S. The calculated O-O, C-O, C*-O, N-O, C-C*, and C*-N bond lengths of the N-SWNTs^{Q} for all three adsorption states in Å. Where C* is one of the carbon atoms adjacent to N atom on which oxygen adsorption is considered.

N-SWNT	Physisorption state		Chemisorption state		Dissociative adsorption	
Charge (Q)	0	-1	0	-1	0	-1
(15,0)MZ	Diameter = 11.74 Å					
O-O	1.24	1.24	1.50	1.50	2.80	2.80
C-O	3.67	3.58	1.52	1.52	1.45	1.46
C*-O	3.45	3.94 (N-O 3.49)	1.47	1.47	1.43	1.43
C-C*	1.41	1.41	1.53	1.53	1.49	1.49
C*-N	1.41	1.41	1.48	1.48	1.465	1.465
(18,0)MZ	Diameter = 14.09 Å					
O-O	1.24	1.24	1.50	1.50	2.67	2.67
C-O	3.61	3.62	1.52	1.52	1.43	1.43
C*-O	3.33	3.65 (N-O 3.45)	1.47	1.47	1.24	1.24
C-C*	1.42	1.42	1.53	1.53	1.53	1.53
C*-N	1.41	1.41	1.48	1.48	2.10	2.07
(21,0)MZ	Diameter = 16.4406 Å					
O-O	1.24	1.24	1.50	1.50	2.79	2.79
C-O	3.56	3.71	1.52	1.53	1.45	1.46
C*-O	3.23	3.28	1.47	1.48	1.43	1.43
C-C*	1.42	1.42	1.53	1.53	1.49	1.49
C*-N	1.41	1.41	1.48	1.48	1.47	1.47
(16,0)SZ	Diameter = 12.53 Å					
O-O	1.25	1.25	1.50	1.50	2.73	2.68
C-O	3.20	3.61	1.53	1.53	1.42	1.42
C*-O	3.07	3.23	1.48	1.47	1.35	1.24

C-C*	1.41	1.41	1.54	1.53	1.53	1.52
C*-N	1.42	1.42	1.48	1.48	1.56	2.12
(17,0)SZ	Diameter = 13.25 Å					
O-O	1.24	1.25	1.50	1.50	2.68	2.68
C-O	3.76	3.61	1.52	1.53	1.42	1.43
C*-O	3.76	4.14 (N-O 3.71)	1.47	1.48	1.24	1.24
C-C*	1.41	1,42	1.53	1.53	1.53	1.53
C*-N	1.40	1.41	1.48	1.48	2.11	2.10
(19,0)SZ	Diameter = 14.91 Å					
O-O	1.24	1.24	1.50	1.50	2.80	2.80
C-O	3.69	3.84	1.52	1.55	1.45	1.46
C*-O	3.64	3.51	1.47	1.47	1.42	1.42
C-C*	1.42	1.42	1.53	1.53	1.49	1.49
C*-N	1.41	1.41	1.48	1.48	1.47	1.47
(20,0)SZ	Diameter = 15.66 Å					
O-O	1.24	1.25	1.50	1.50	2.79	2.79
C-O	3.72	3.75	1.53	1.54	1.46	1.45
C*-O	3.28	3.30	1.47	1.48	1.42	1.42
C-C*	1.42	1.42	1.53	1.53	1.49	1.49
C*-N	1.41	1.41	1.48	1.48	1.47	1.47
(9,9)MA	Diameter = 12.204 Å					
O-O	1.25	1.26	1.50	1.49	2.81	2.84
C-O	3.32	3.07	1.52	1.59	1.45	1.45
C*-O	3.23	2.96	1.47	1.50	1.25	1.28
C-C*	1.41	1.42	1.57	1.56	1.56	1.57
C*-N	1.41	1.41	1.46	1.45	1.88	1.72
(10,10)MA	Diameter = 13.56 Å					

O-O	1.25	1.26	1.50	1.49	3.02	2.83
C-O	3.30	3.89	1.53	1.59	1.46	1.45
C*-O	3.06	3.67	1.47	1.50	1.42	1.27
C-C*	1.41	1.42	1.57	1.56	1.46	1.57
C*-N	1.41	1.41	1.46	1.45	1.46	1.73
(11,11)MA		Diameter = 14.916 Å				
O-O	1.25	1.28	1.50	1.49	3.04	2.81
C-O	3.31	3.12	1.53	1.59	1.46	1.45
C*-O	3.23	3.09 (N-O 2.92)	1.47	1.50	1.42	1.28
C-C*	1.41	1.42	1.57	1.56	1.52	1.57
C*-N	1.41	1.41	1.46	1.45	1.46	1.72
(12,12)MA		Diameter = 16.272 Å				
O-O	1.25	1.26	1.50	1.49	2.76	2.80
C-O	3.36	3.18	1.53	1.59	1.44	1.45
C*-O	3.06	2.99	1.47	1.50	1.26	1.27
C-C*	1.41	1.42	1.57	1.56	1.56	1.57
C*-N	1.41	1.41	1.46	1.45	1.86	1.73

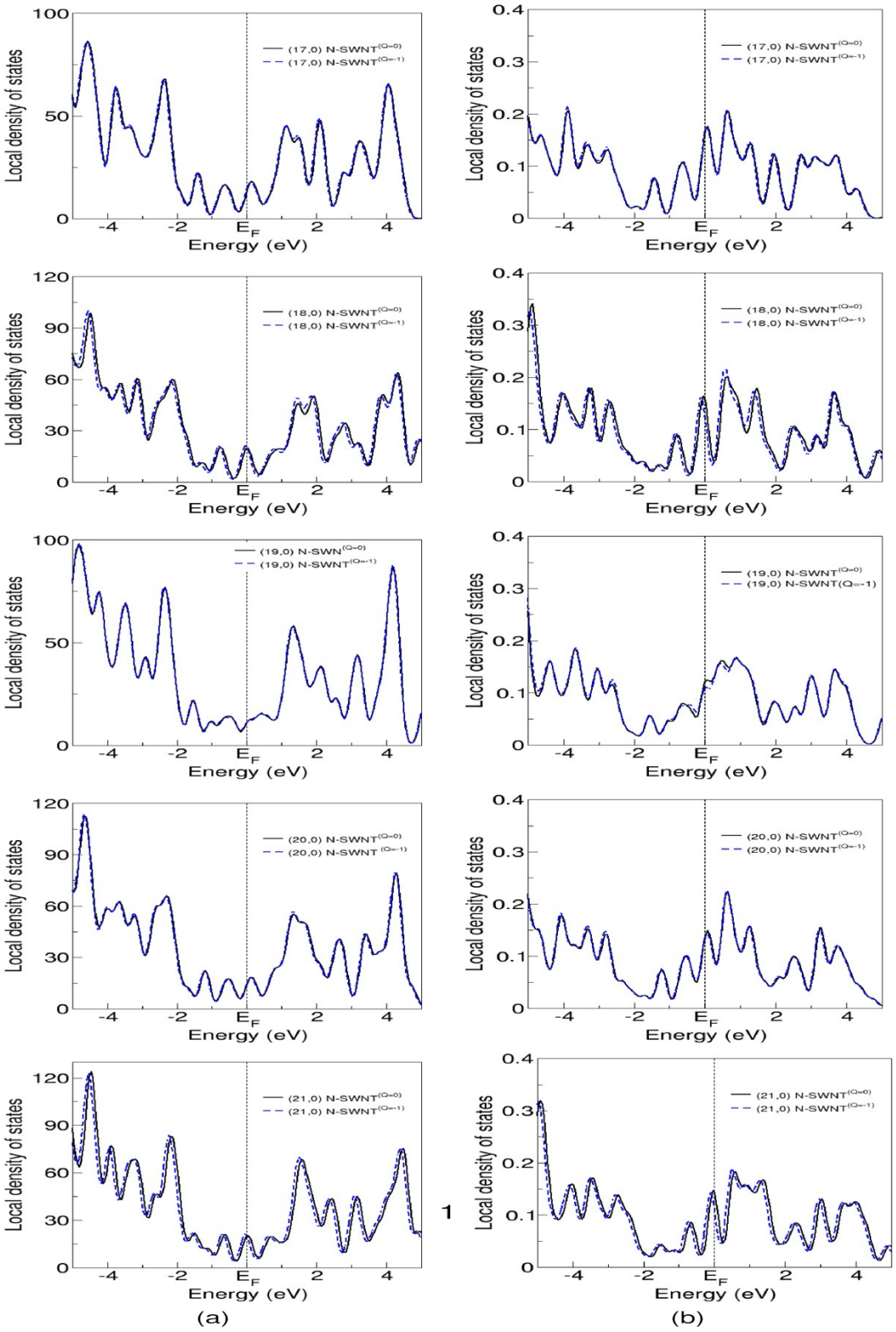

FIG. S1. Local density of states of zigzag N-SWNTs$^{(Q = -1 \text{ and } 0)}$ (a) all C atoms, and (b) a N atom. E_F represents the Fermi level.

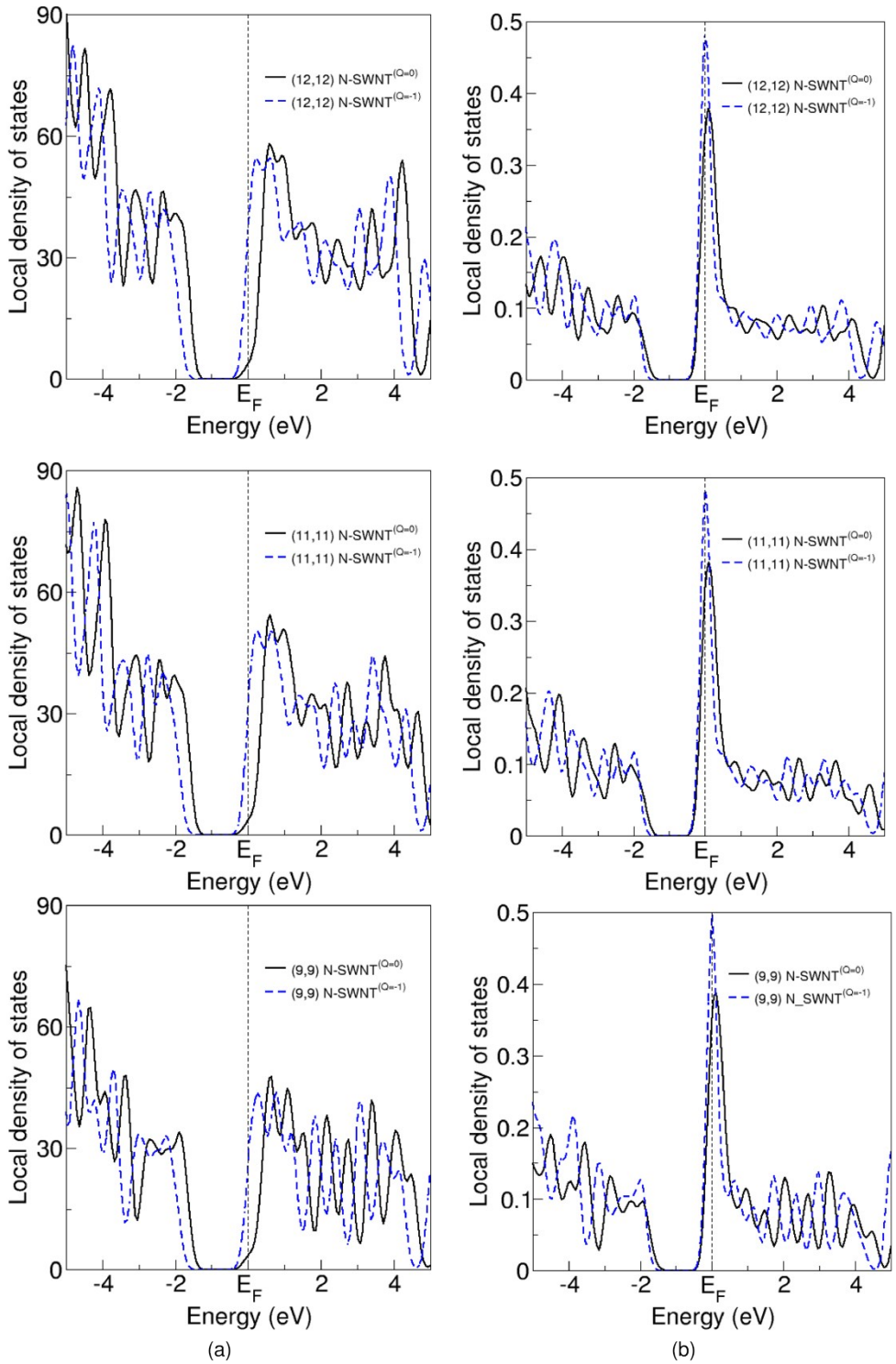

FIG. S2. Local density of states of armchair N-SWNTs$^{(Q = -1 \text{ and } 0)}$ (a) all C atoms, and (b) a N atom. E_F represents the Fermi