Supplementary Information

Encapsulated aluminum nanoparticles into carbon nanotubes for combustion: A molecular dynamics study

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In order to verify the adequacy of the ReaxFF potential for the title composite, the bond parameters of the interaction between CNTs and ANPs were calculated and shown in Fig. S1 and Table S1. The bond parameters were calculated using ReaxFF and DFT method (GGA/PBE functional in Dmol^3 module). As can be seen from Table S1, the bond parameters optimized by ReaxFF force fields are excellently consistent with those by DFT method.

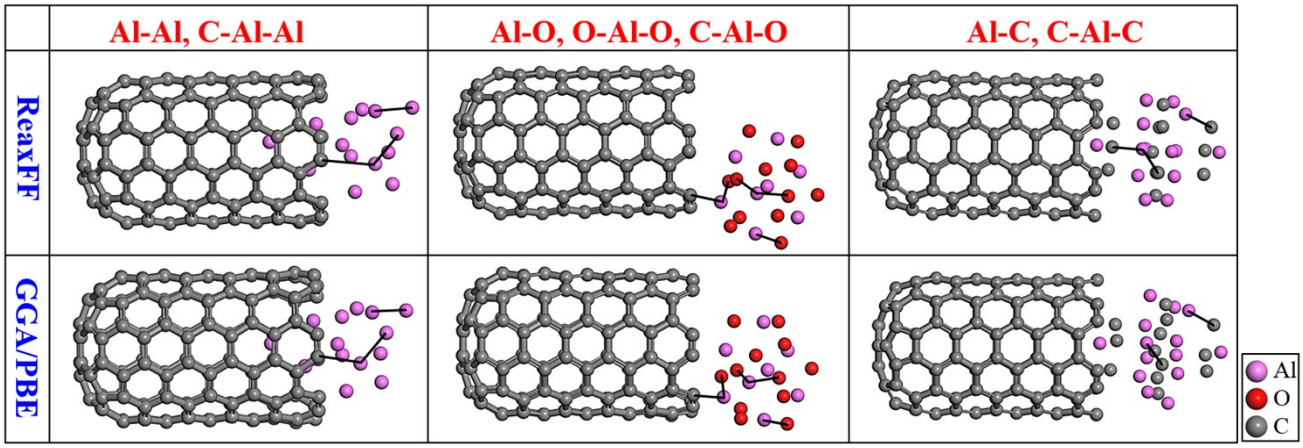

Fig. S1 The optimized structure of CNTs/ANPs composites by ReaxFF and DFT methods. The black line represents the sampled bond length and bond angle.

Table S1 Bond parameters of Al-X (X=C/O) interactions. The bond lengths (L, Å), bond angles (A, °), bond/angle energies (E, kcal/mol), and relative error (Er, %) of the Al-X (X=C/O) interactions for CNTs/ANPs composite.

Bond	No.	Bond type	L_{ReaxFF}	$L_{GGA/PBE}$	Er (%)	E_{ReaxFF}	$E_{GGA/PBE}$	Er (%)

	1	Al-C	1.87	1.91	2.09	109.11	112.53	3.04
	2	Al-O	1.81	1.77	−2.26	171.12	169.97	−0.68
	3	Al-Al	2.64	2.74	3.65	75.58	79.68	5.15
	No.	Angle type	A_{ReaxFF}	$A_{GGA/PBE}$	*Er* (%)	E_{ReaxFF}	$E_{GGA/PBE}$	*Er* (%)
Bond angle	1	C-Al-Al	120.79	124.35	2.86	15.92	15.36	−3.65
	2	C-Al-C	119.32	117.40	−1.64	27.39	25.94	−5.59
	3	C-Al-O	114.48	115.84	1.17	36.98	36.67	−0.85
	4	O-Al-O	115.18	117.63	2.08	38.89	39.01	0.31