

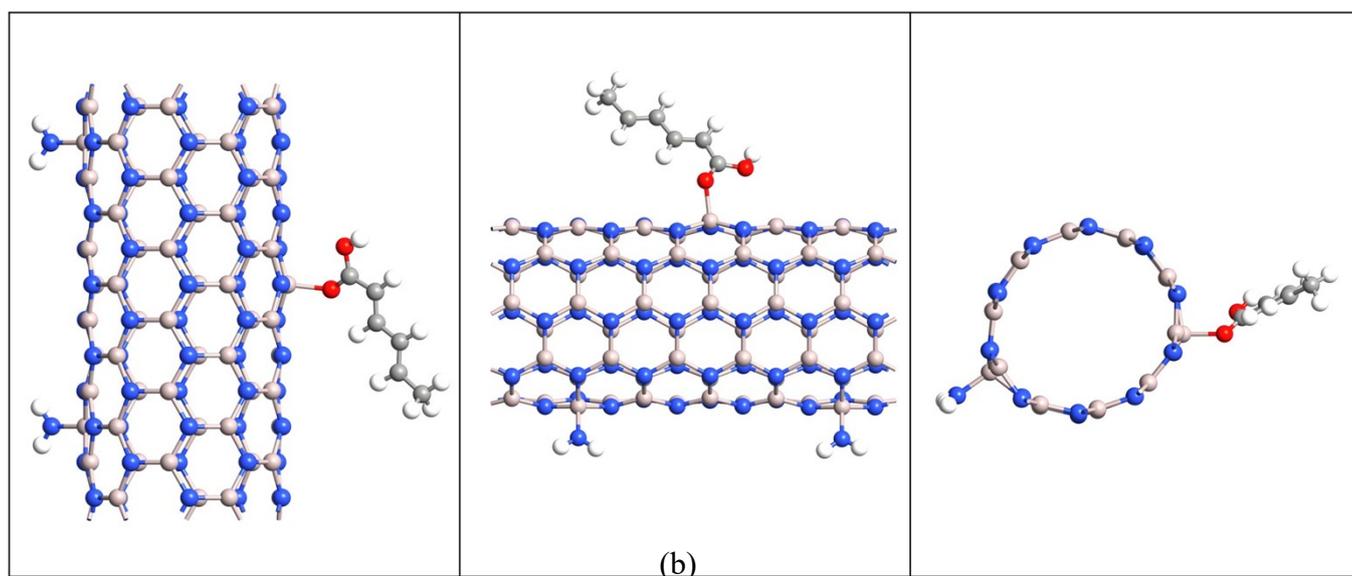
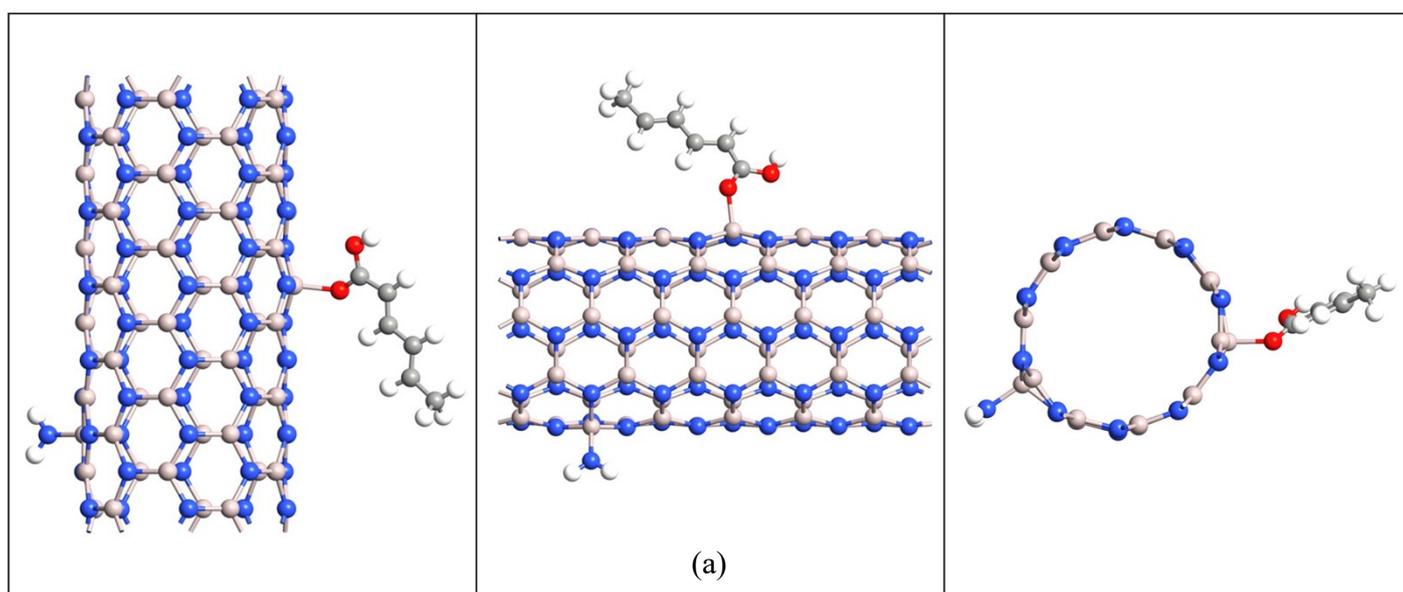
Supplementary Information

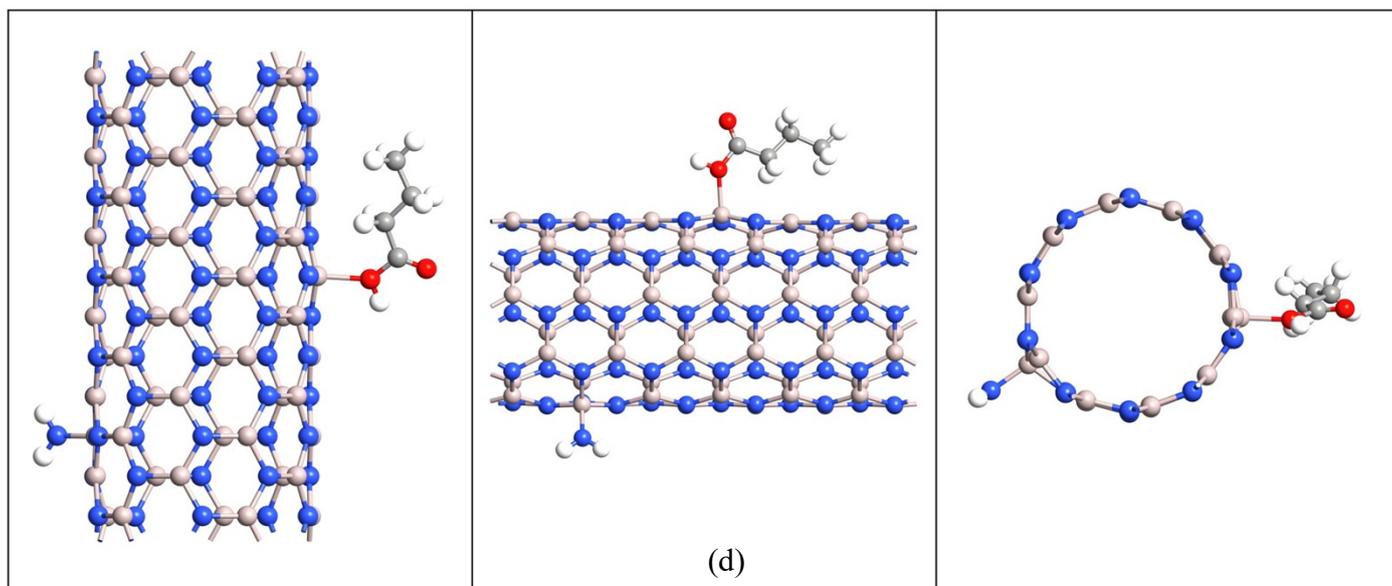
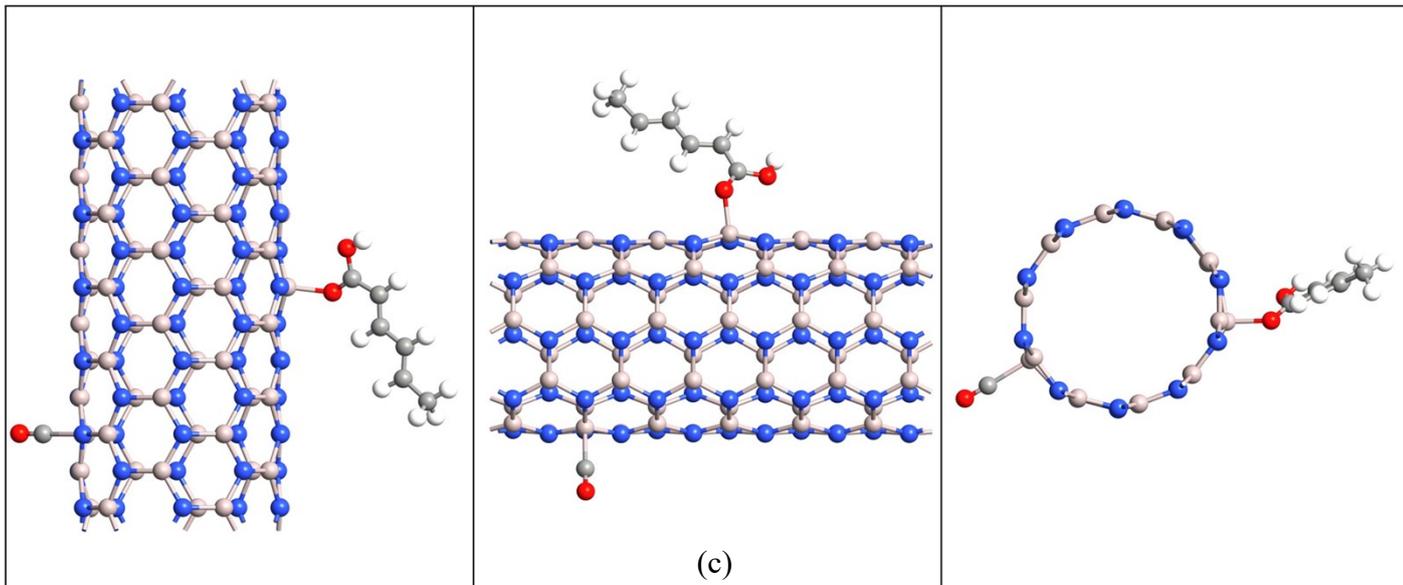
Tailored Surface Functionalization of AlN Nanotubes for 5-Fluorouracil Adsorption and Encapsulation: A First-Principles and Molecular Dynamics Study

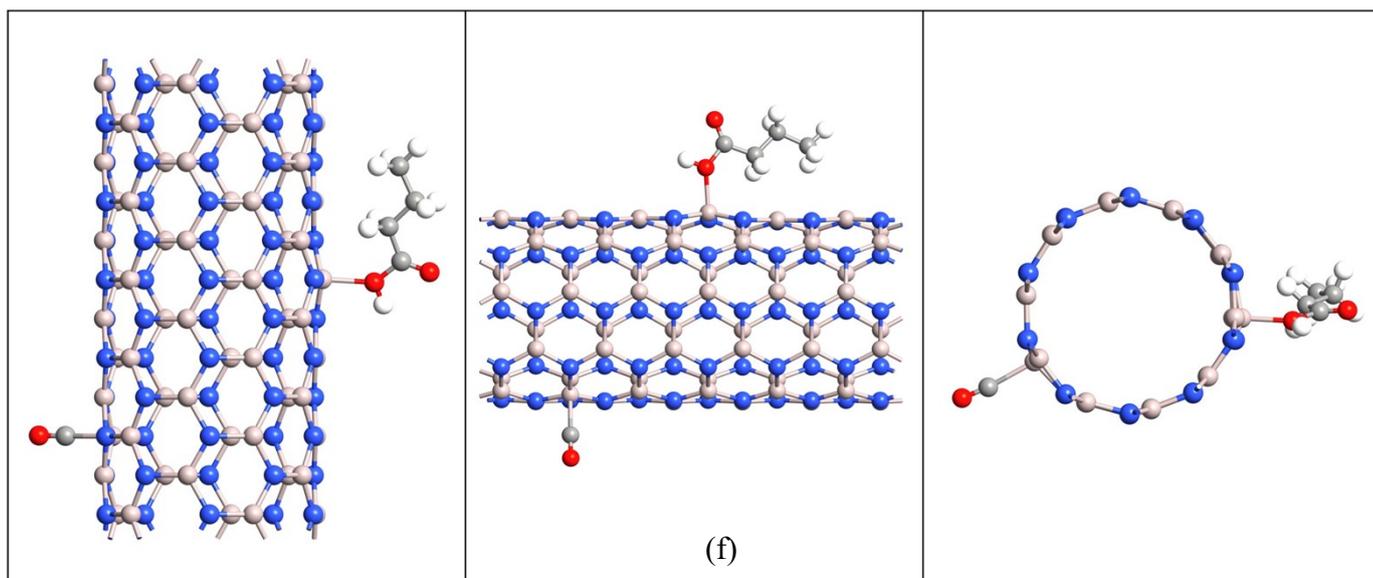
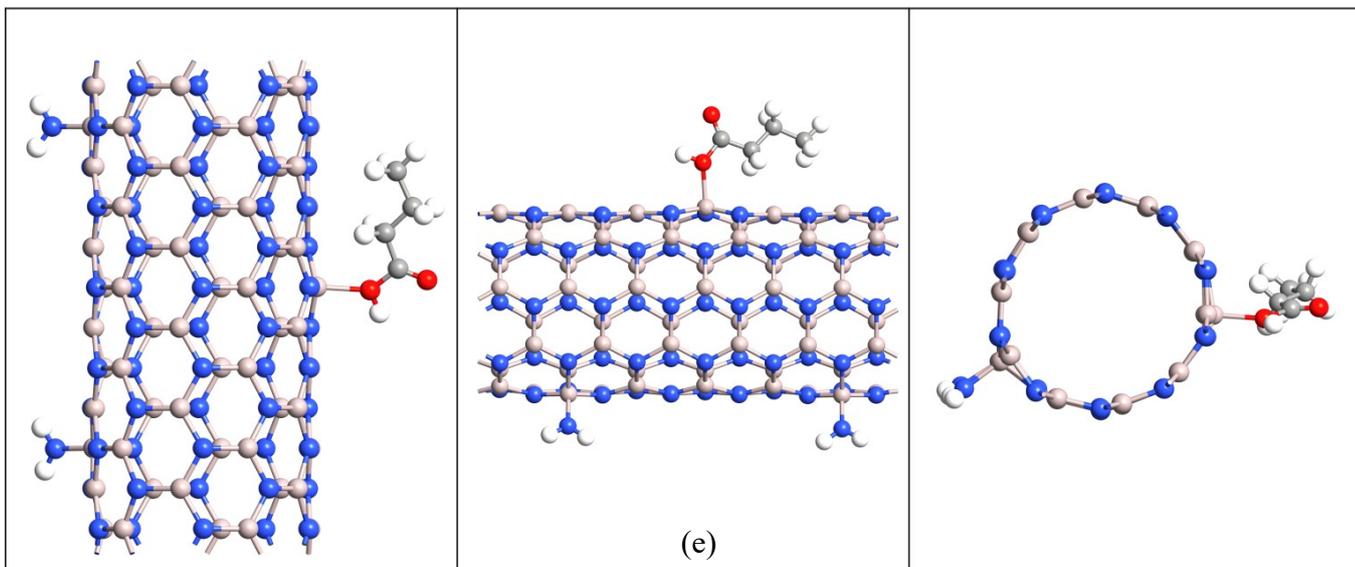
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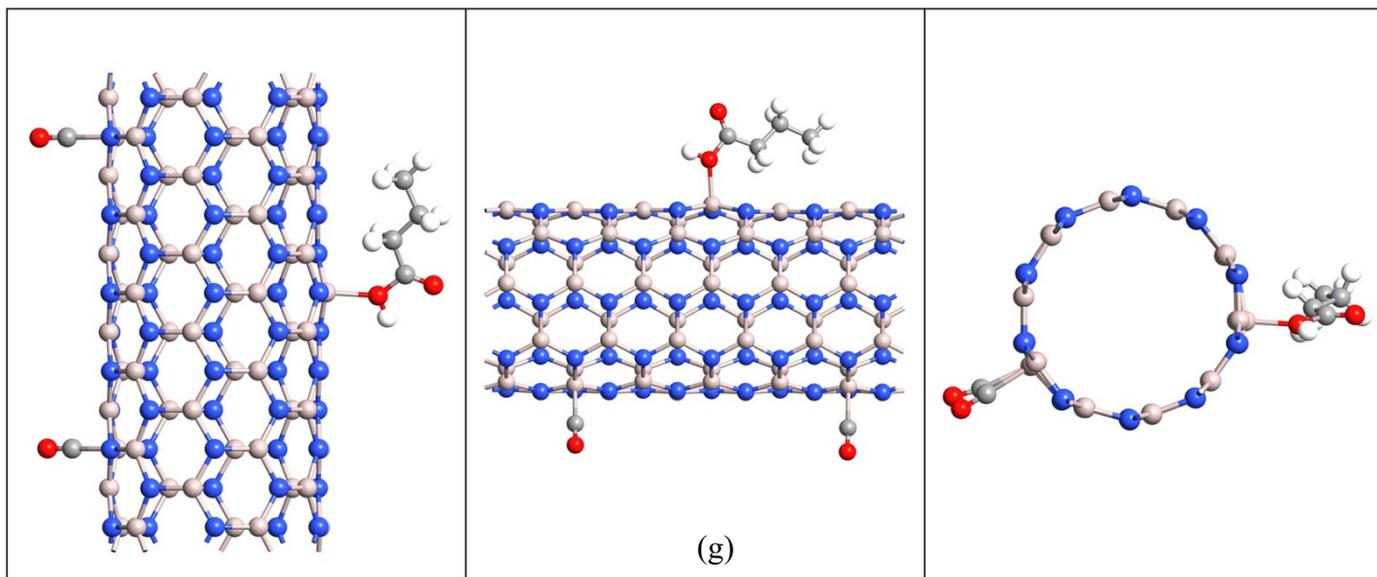


Figure.S1 Optimized side, top, and cross-sectional views of functionalized Aluminum Nitride Nanotube systems (a) AlNNT(SA)(-NH₂), (b) AlNNT(SA)₂(-NH₂), (c) AlNNT(SA)(C=O), (d) AlNNT(BA)(-NH₂), (e) AlNNT(BA)₂(-NH₂), (f) AlNNT(BA)(C=O), and (g) AlNNT(BA)₂(C=O).

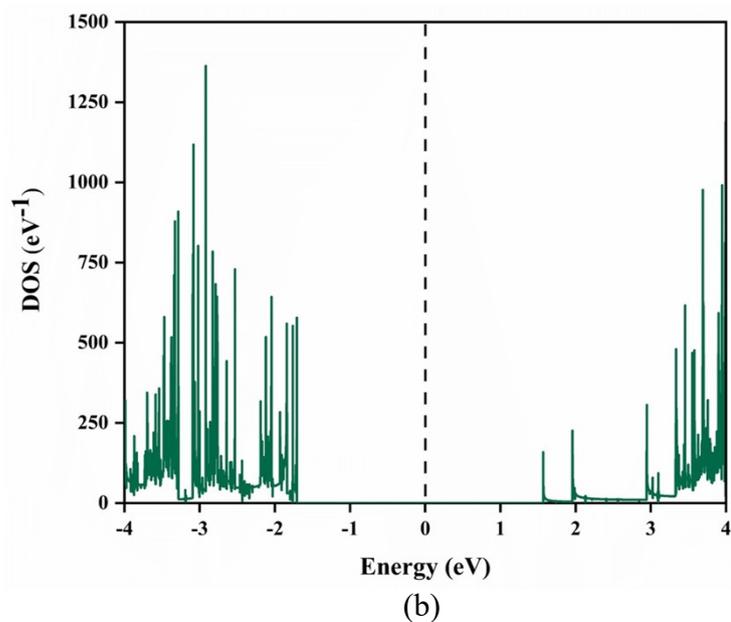
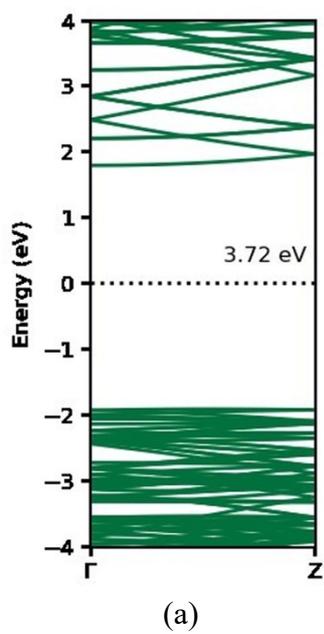


Figure S2: Pristine AlNNT (a) Bandstructure, (b) DOS

Systems	Bond Length (Å)	Bond Angle (°)	s Character (%)	p Character (%)
AlNNT (SA)	1.93	101.48	16.60	83.40
AlNNT (BA)	2.09	98.93	13.44	86.56
AlNNT (SA) (-NH₂)	1.89	104.54	20.07	79.30
AlNNT (SA) 2(-NH₂)	1.87	105.61	21.21	78.79
AlNNT (SA) (C=O)	2.03	99.89	14.66	85.34
AlNNT (SA) 2(C=O)	2.06	98.36	12.70	87.30
AlNNT (BA) (-NH₂)	1.96	103.26	18.66	81.34
AlNNT (BA) 2(-NH₂)	1.92	104.65	20.18	79.82
AlNNT (BA) (C=O)	2.10	98.79	13.26	86.74
AlNNT (BA) 2(C=O)	2.10	98.46	12.83	87.17

Table S1. Bond Length (Å), Bond Angle (°), and hybridization (*s/p* character) (%) of SA- and BA-functionalized AlNNT systems.

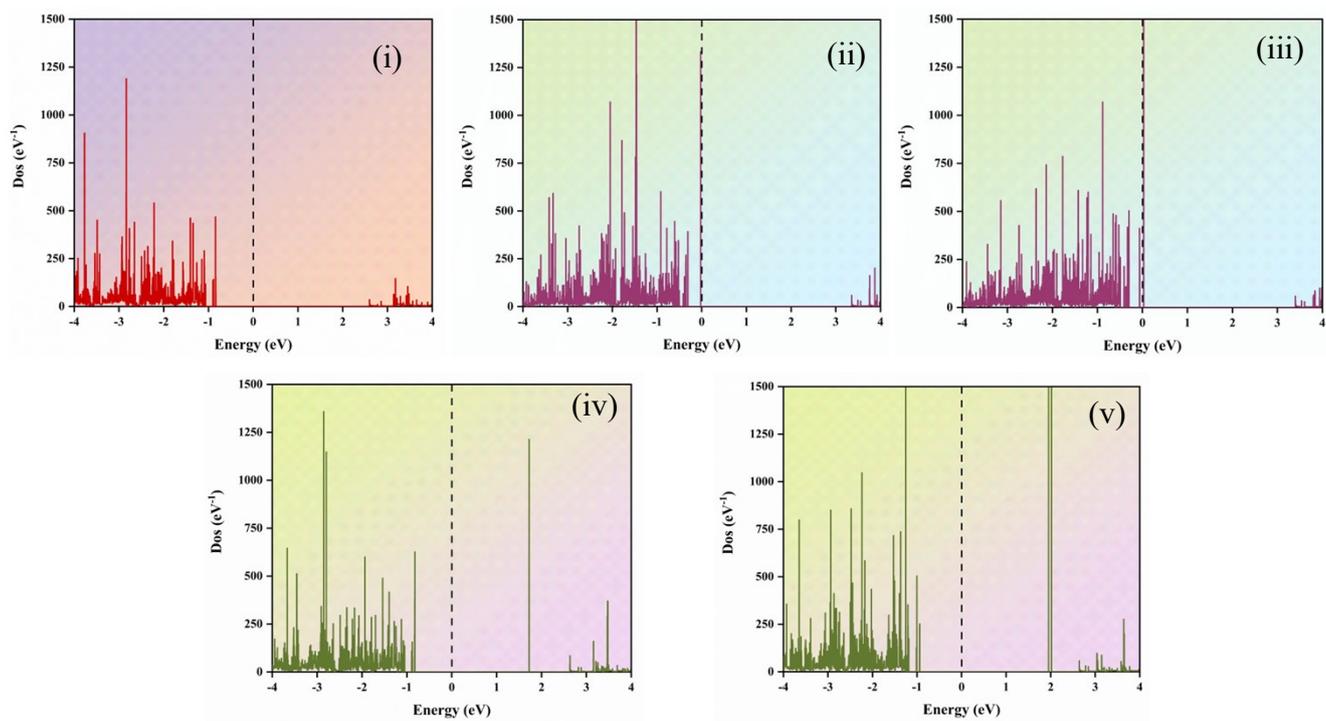


Figure S3a. Density of States for (i)AINNT (SA), (ii)AINNT (SA)(-NH₂), (iii)AINNT (SA)₂(-NH₂), (iv)AINNT (SA)(C=O), and (v)AINNT (SA)₂(C=O).

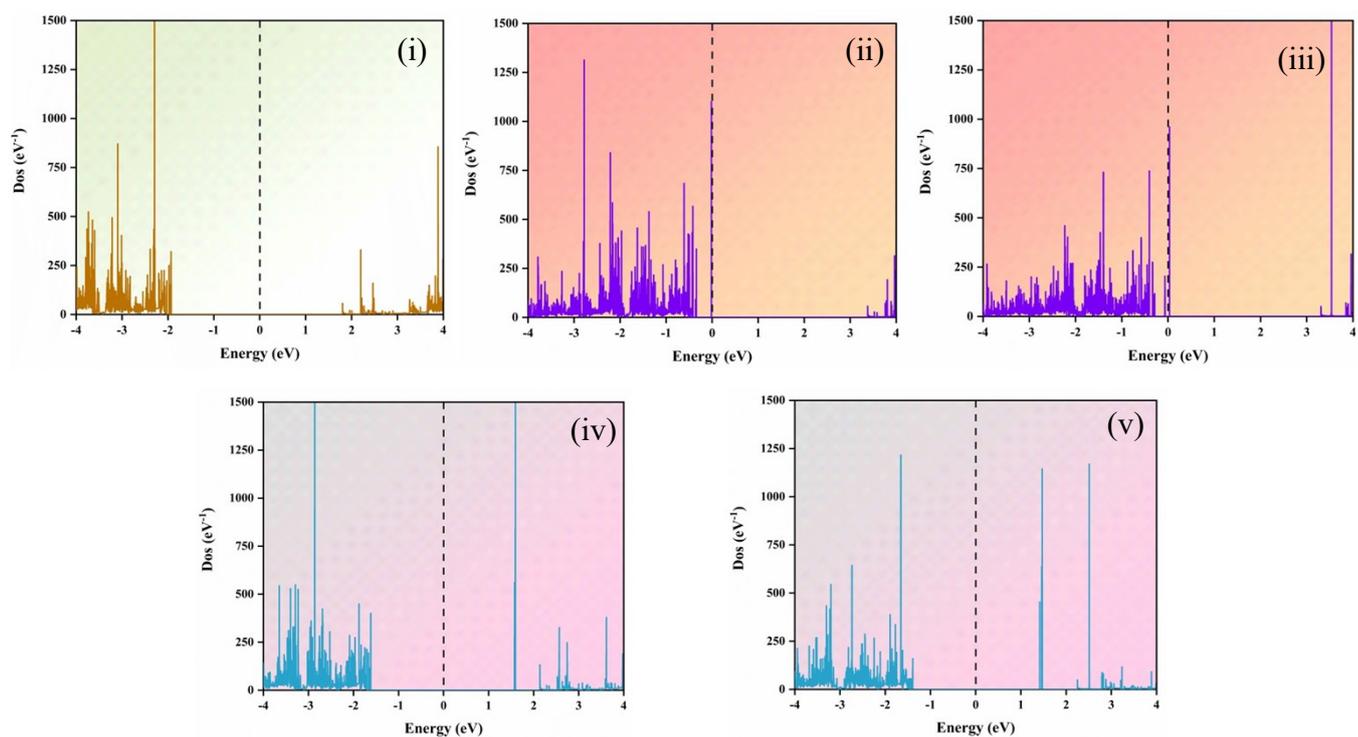


Figure S3b. Density of States for (i)AINNT (BA), (ii)AINNT (BA)(-NH₂), (iii)AINNT (BA)₂(-NH₂), (iv)AINNT (BA)(C=O), and (v)AINNT (BA)₂(C=O).

Systems	Binding Energy (eV)	Formation Energy (eV)
AINNT (SA)	-2.05	-7.76
AINNT (BA)	-1.67	-10.27
AINNT (SA) (-NH₂)	-4.65	-7.01
AINNT (SA) 2(-NH₂)	-7.25	-7.01
AINNT (SA) (C=O)	-3.10	-7.11
AINNT (SA) 2(C=O)	-4.13	-7.12
AINNT (BA) (-NH₂)	-4.22	-7.03
AINNT (BA) 2(-NH₂)	-6.78	-6.99
AINNT (BA) (C=O)	-2.69	-7.08
AINNT (BA) 2(C=O)	-3.31	-7.09

Table S2. Binding Energy (eV) and Formation Energy (eV) of SA- and BA-functionalized AINNT systems.

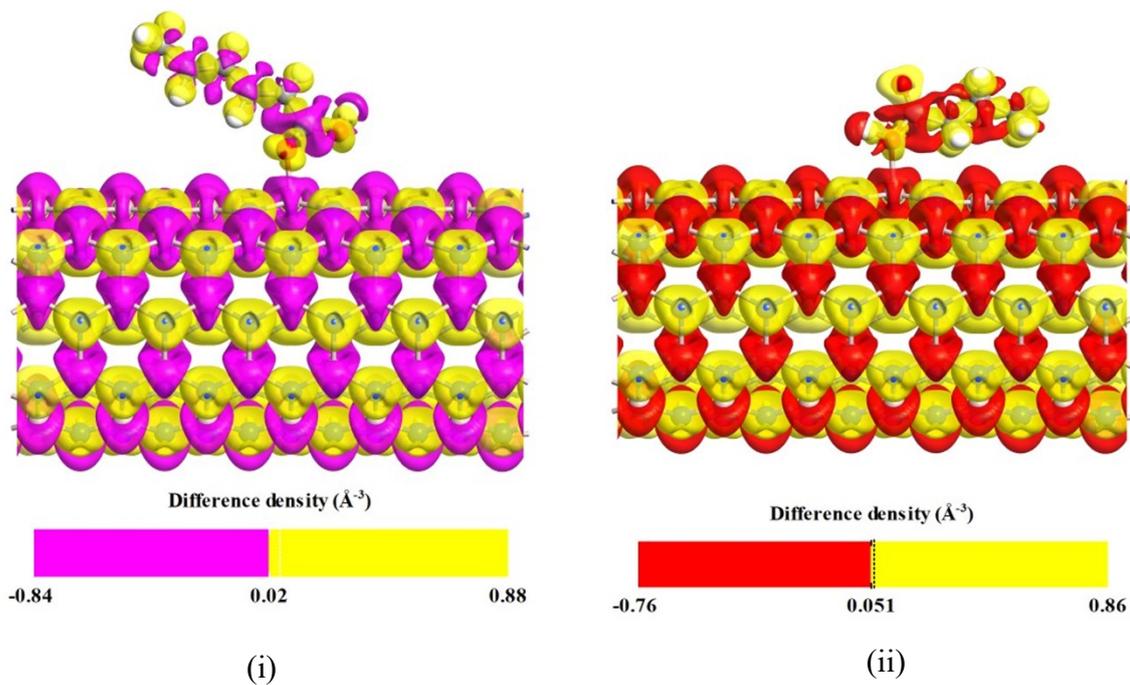
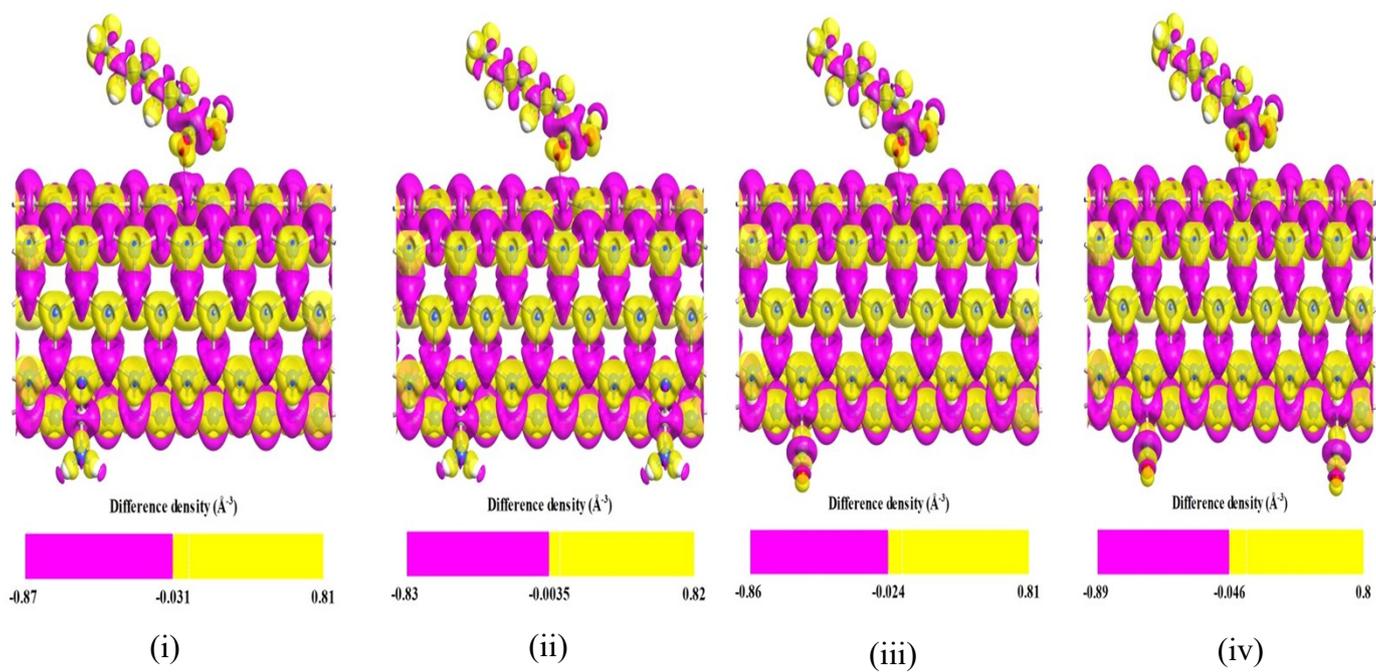


Figure S4a. EDD for (i)AINNT (SA), and (ii)AINNT



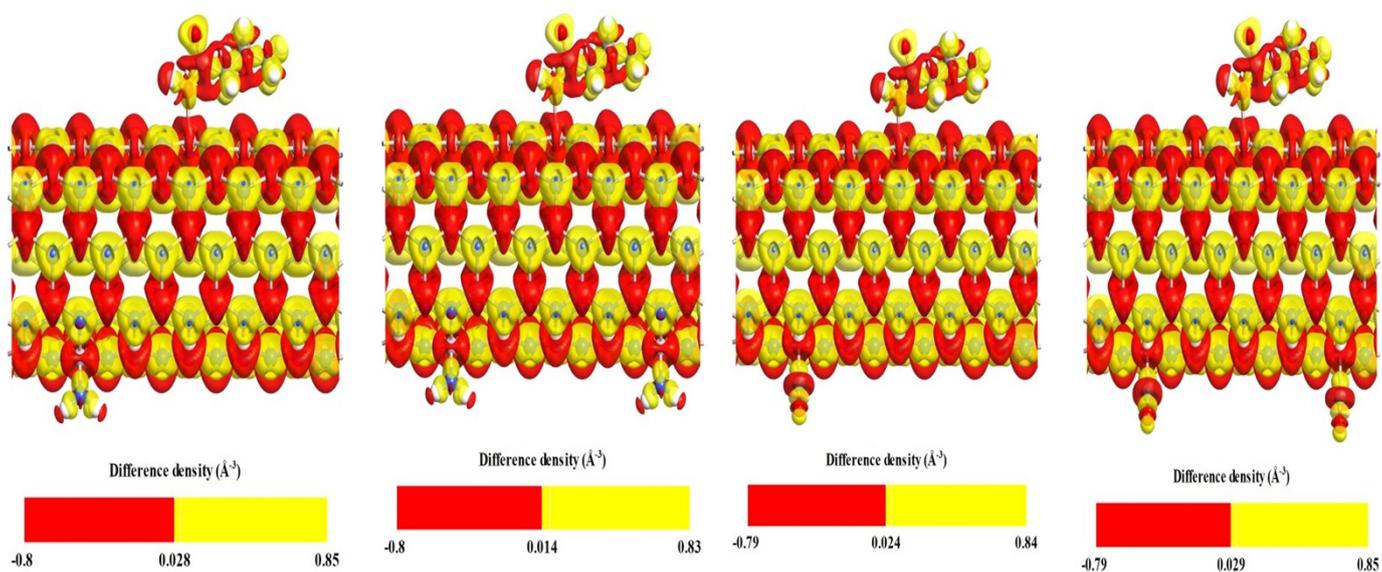


Figure S4b. EDD for (i) AINNT (SA)(-NH₂), (ii) AINNT (SA)₂(-NH₂), (iii) AINNT (SA)(C=O), and (iv) AINNT (SA)₂(C=O)

Figure S4c. EDD for (i) AINNT (BA)(-NH₂), (ii) AINNT (BA)₂(-NH₂), (iii) AINNT (BA)(C=O), and (iv) AINNT (BA)₂(C=O)