Electronic Supplementary Information

Graphyne Nanotubes as Promising Sodium-Ion Battery Anodes

Yuan Yuan [a, #], Xiaoxue Song [b, #], Jiapeng Ma [a], Yanqi Chen [a], Fang-Fang Wang [a], Baotao Kang [a, b, *] and Jin Yong Lee [b, *]

[a] School of Chemistry and Chemical Engineering, University of Jinan, Jinan, Shandong 250022, P. R. China

E-mail: chm_kangbt@ujn.edu.cn

[b] Department of Chemistry, Sungkyunkwan University, Suwon, 16419, Republic of Korea

E-mail: jinylee@skku.edu

Table of contents

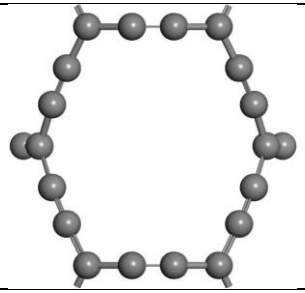
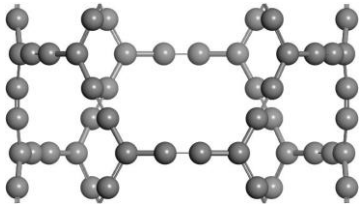
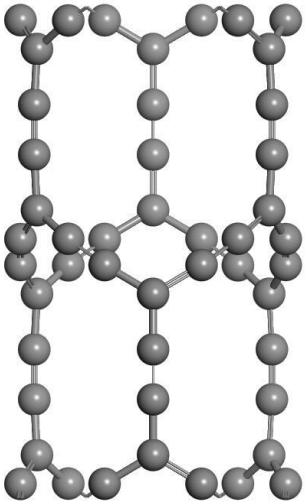
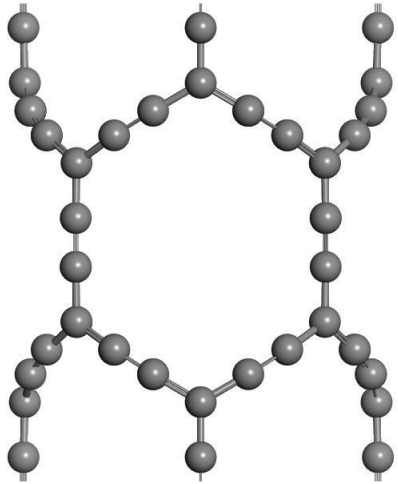
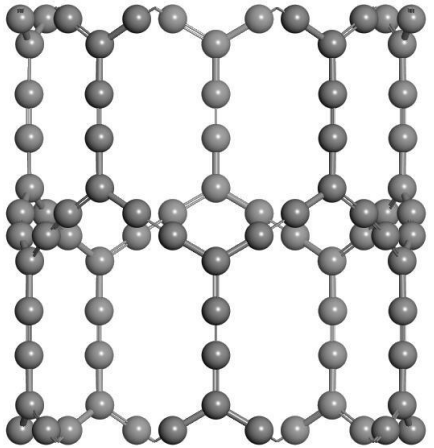
n	2	3	4	5
(*n*, *n*)				\
(*n*, 0)	\			

Figure S 1 Optimized structure of all studied αGyNTs.

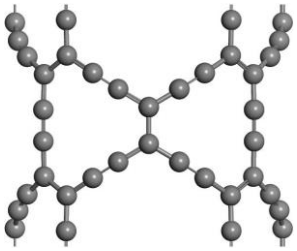
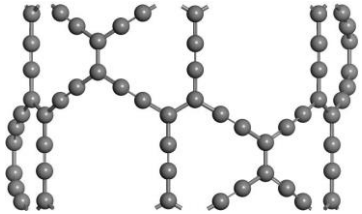
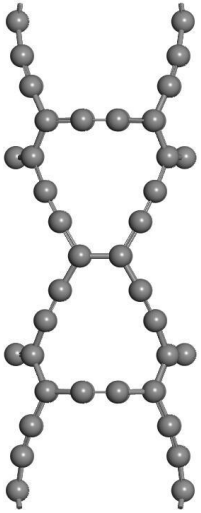
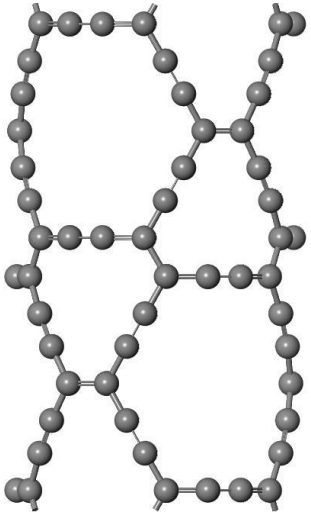
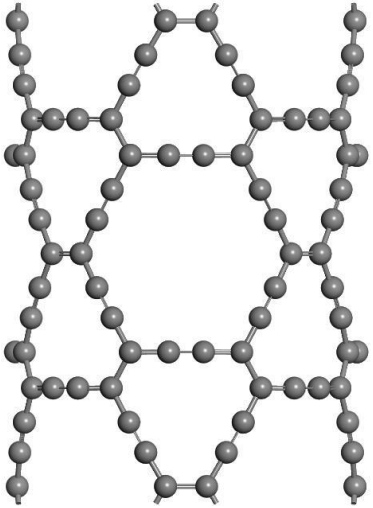
n	2	3	4
(*n*, *n*)			
(*n*, 0)			

Figure S 2 Optimized structure of all studied βGyNTs.

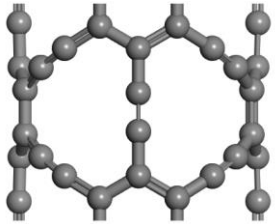
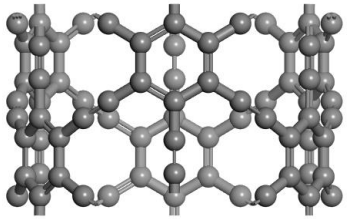
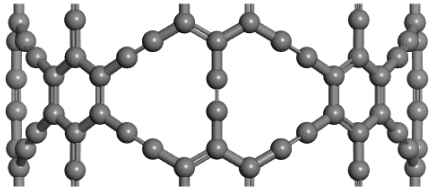
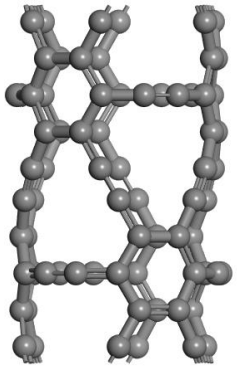
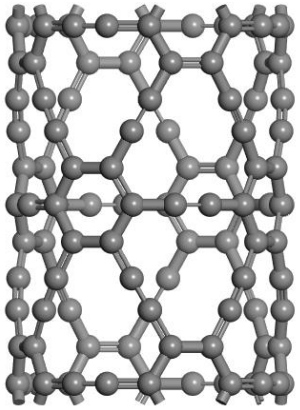
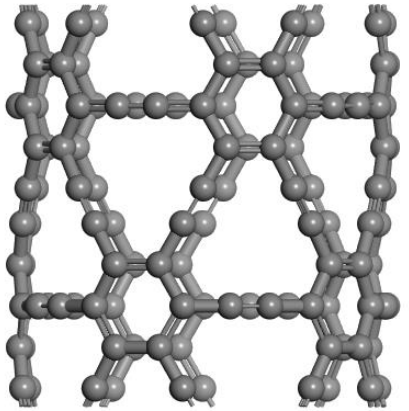
n	2	3	4	5
(*n*, *n*)				\
(*n*, 0)	\			

Figure S 3 Optimized structure of all studied γGyNTs.

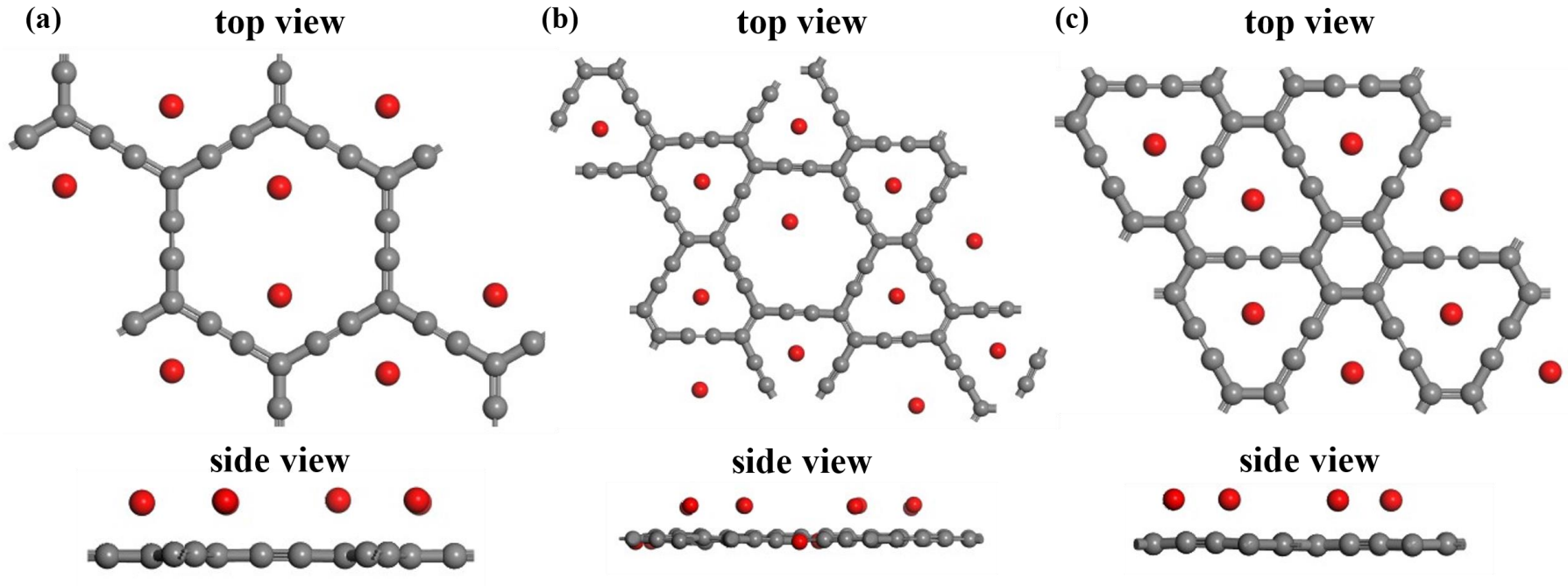


Figure S 4 Optimized structure of αGy (a), βGy (b) and γGy (c) when reaching the maximum storage Na capacities.

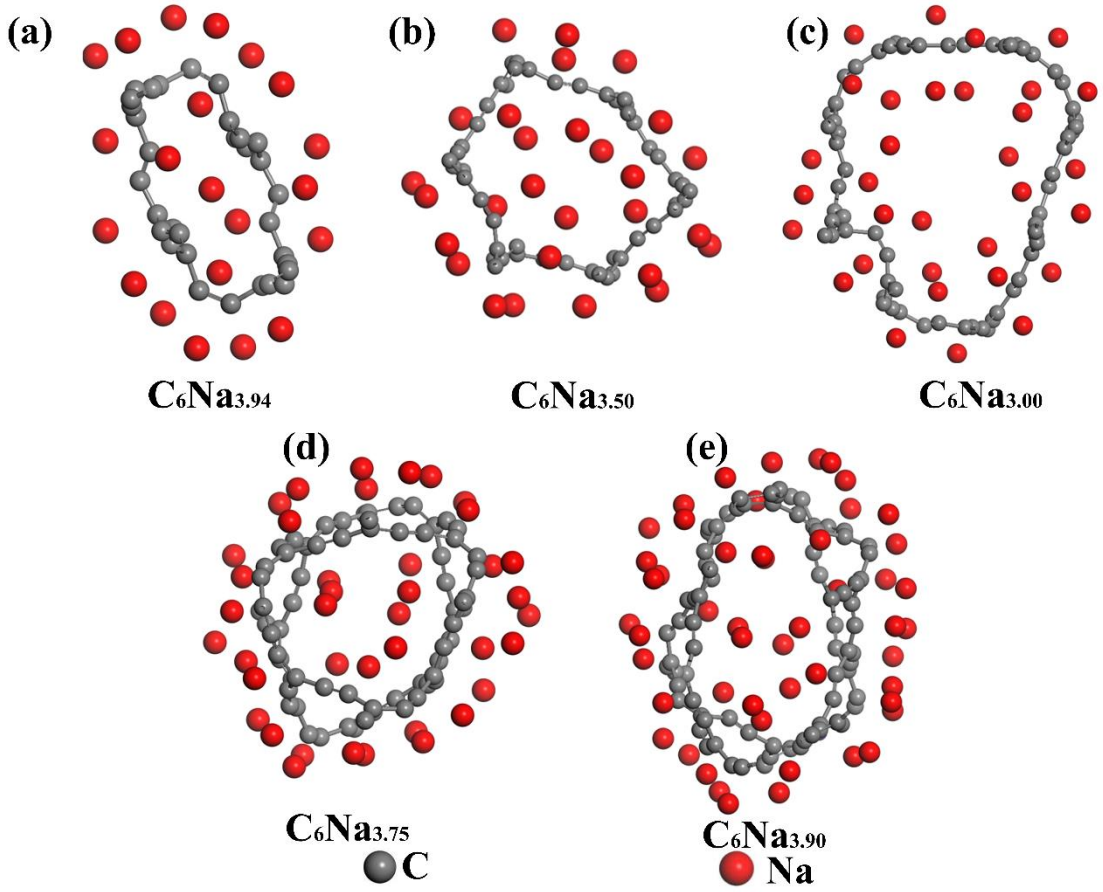


Figure S 5 Optimized geometries with maximum storage capacity of (a) (2, 2)-αGyNT, (b) (3, 3)-αGyNT, (c) (4, 4)-αGyNT, (d) (4, 0)-αGyNT, (e) (5, 0)-αGyNT.

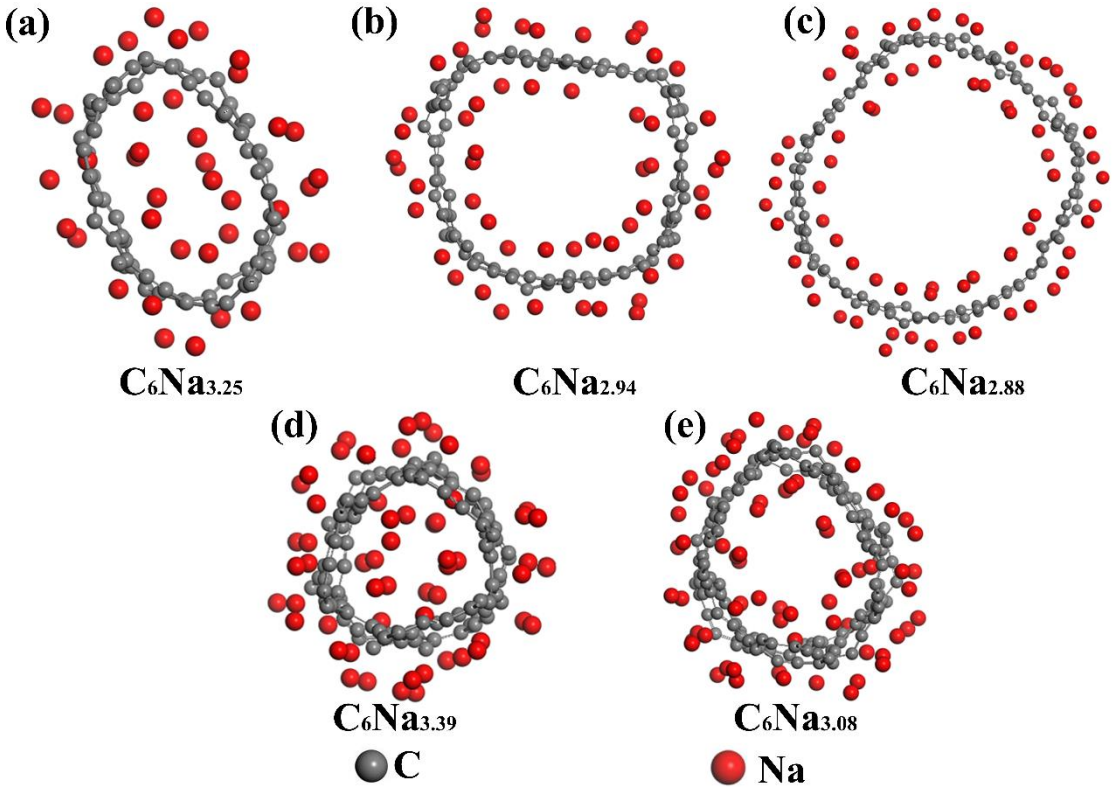


Figure S 6 Optimized geometries with maximum storage capacity of (a) (2, 2)- βGyNT, (b) (3, 3)- βGyNT, (c) (4, 4)- βGyNT, (d) (3, 0)- βGyNT, (e) (4, 0)- βGyNT.

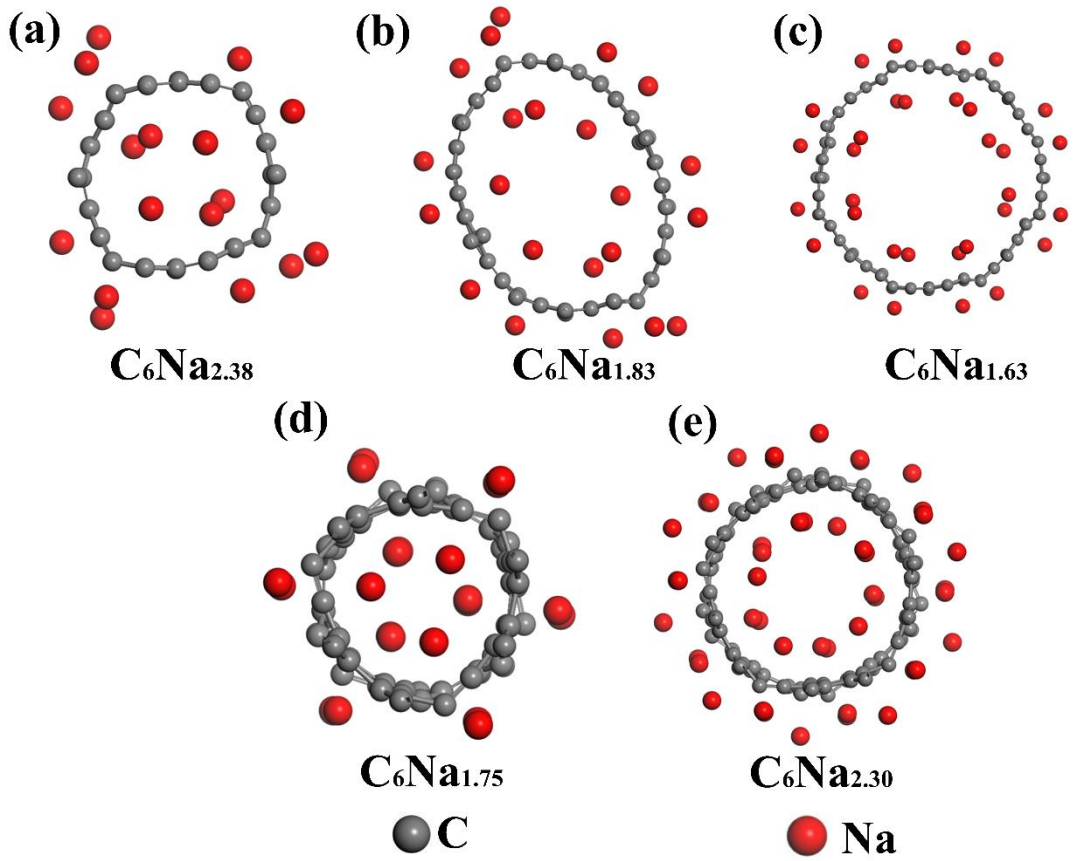


Figure S 7 Optimized geometries with maximum storage capacity of (a) (2, 2)-γGyNT, (b) (3, 3)- γGyNT, (c) (4, 4)- γGyNT, (d) (3, 0)- γGyNT, (e) (5, 0)- γGyNT.

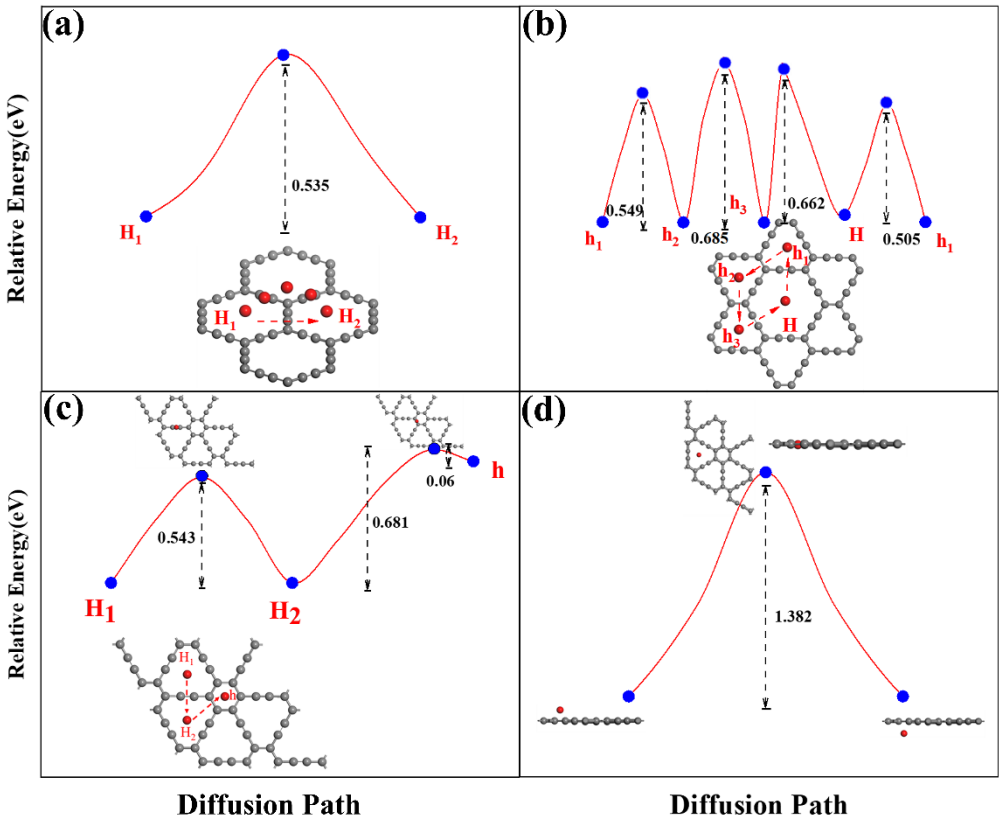


Figure S 8 Energy surfaces of Na diffusion on (a) αGy, (b) βGy, (c) γGy, and Na penetrates on (d) γGy.