Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Structural Transition Induced by Compression and Stretching of Puckered Arsenene Nanotubes

J. J. Quijano-Briones,[a] H. N. Fernández-Escamilla,[*b] J. Guerrero-Sánchez,[b] E. Martínez-Guerra,[a] and Noboru Takeuchi.[b]

[a]CICFIM Facultad de Ciencias Físico Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, N.L. 66450, México.

[b]Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Apartado Postal 14, Ensenada Baja California, Código Postal 22800, México.

Table of contents

Fig. S1 Charge density isosurfaces for the (19, 0) zigzag nanotube with different lattice vector ……..S2

Fig. S2 Charge density isosurfaces for the (0, 19) armchair nanotube with different lattice vector …..S3

Fig. S3 Electronic band structure for the compressed (9, 0) nanotube…….....S4

Fig. S4 Electronic band structure for the stretched (0, 9) nanotube ……..……..S5

Fig. S5 Electronic band structure for the compressed (14, 0) nanotube …….……...……..S6

Fig. S6 Electronic band structure for the stretched (0, 14) nanotube ……...S7

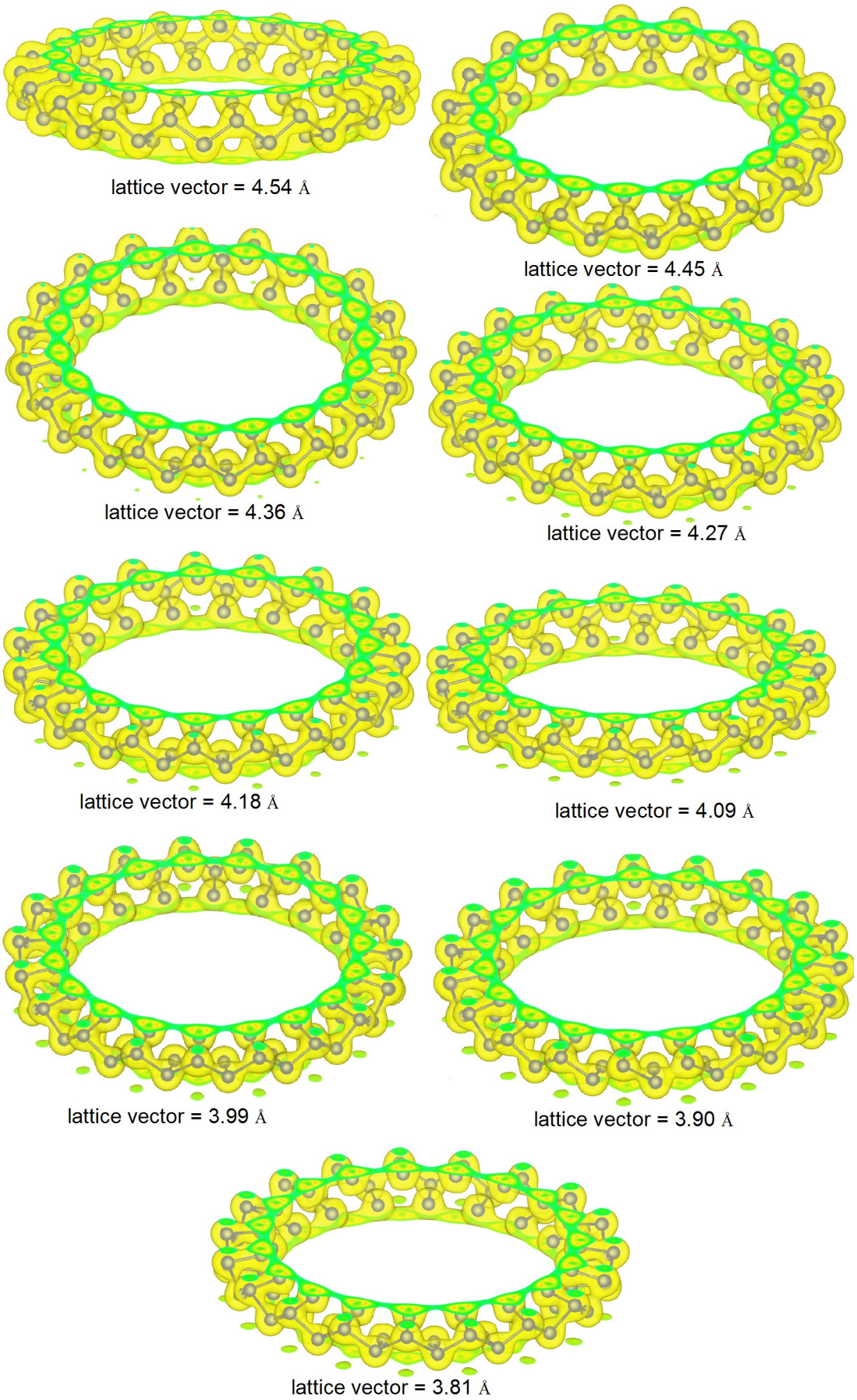

Fig. S1 Charge density isosurfaces for the (19, 0) zigzag nanotube with different lattice vector.

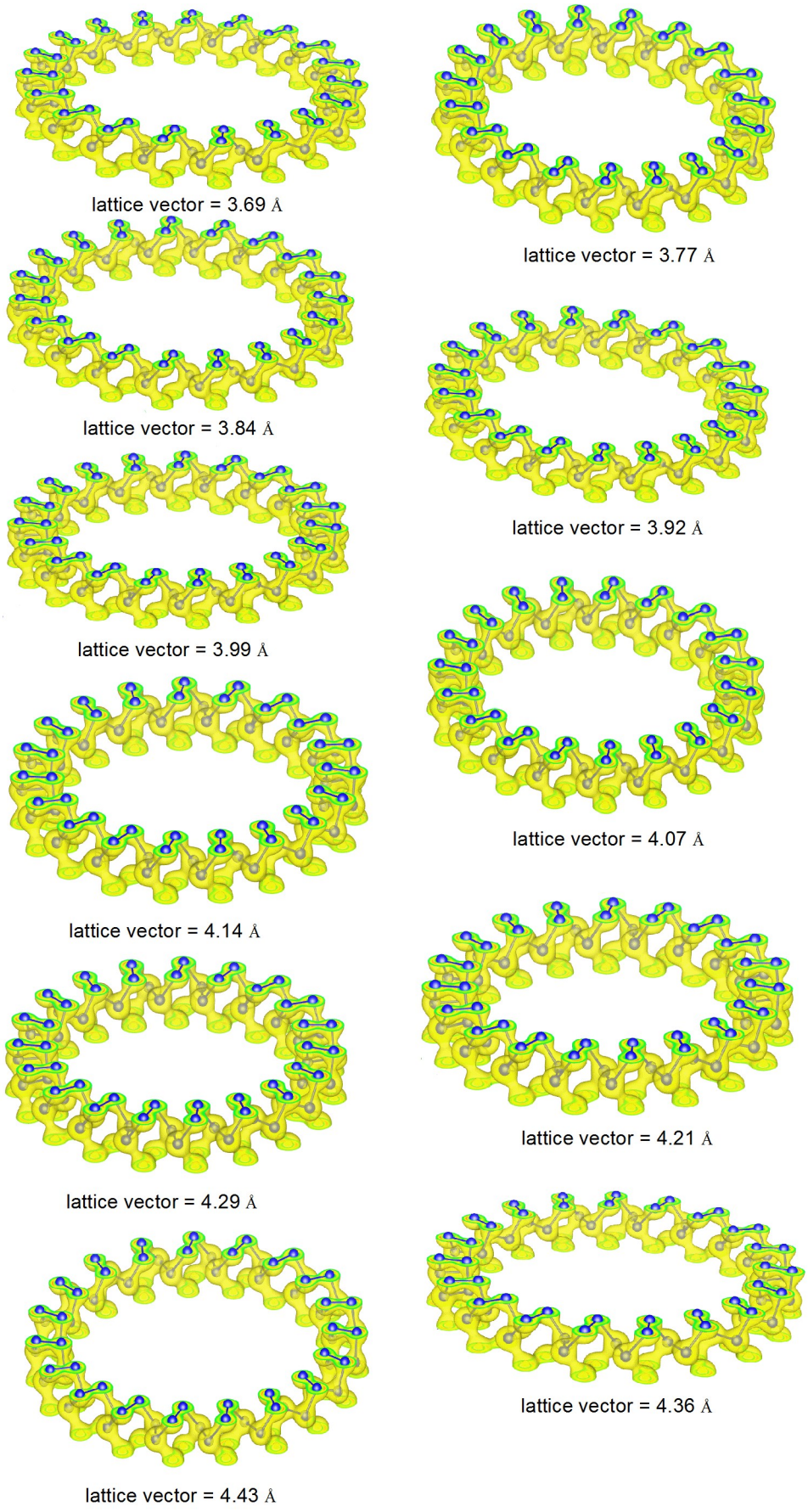

Fig. S2 Charge density isosurfaces for the (0, 19) armchair nanotube with different lattice vector.

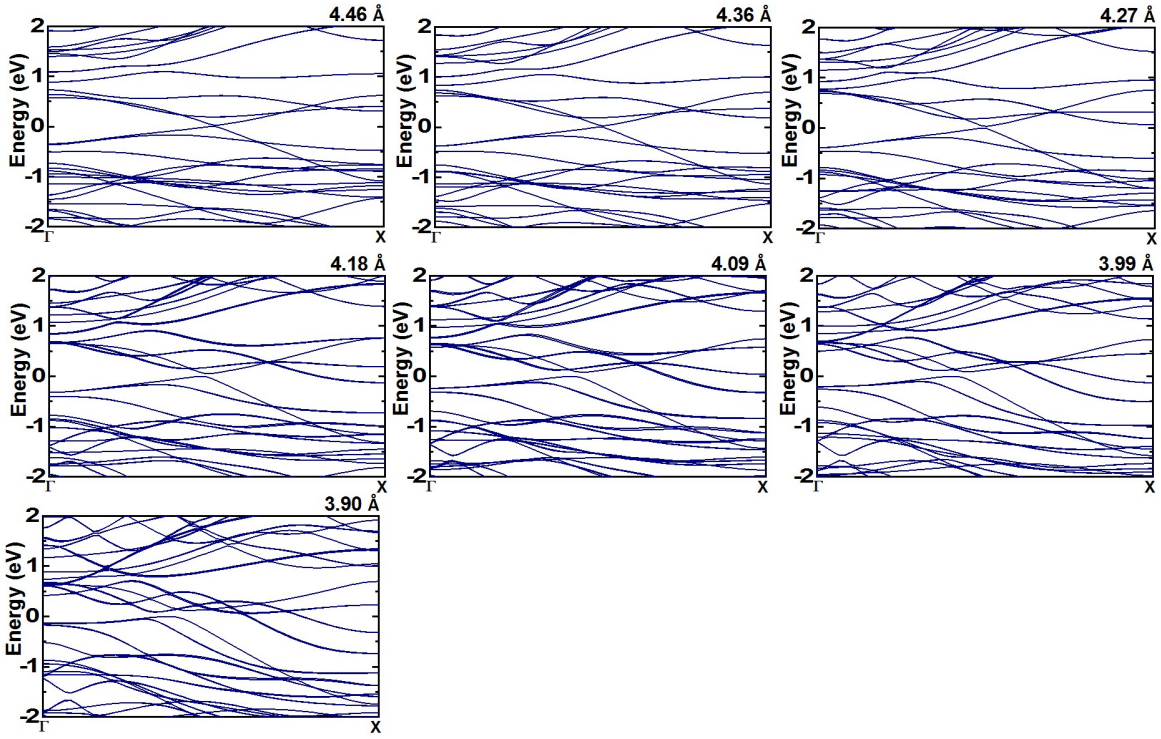

Fig. S3 Electronic band structure for the compressed (9, 0) nanotube.

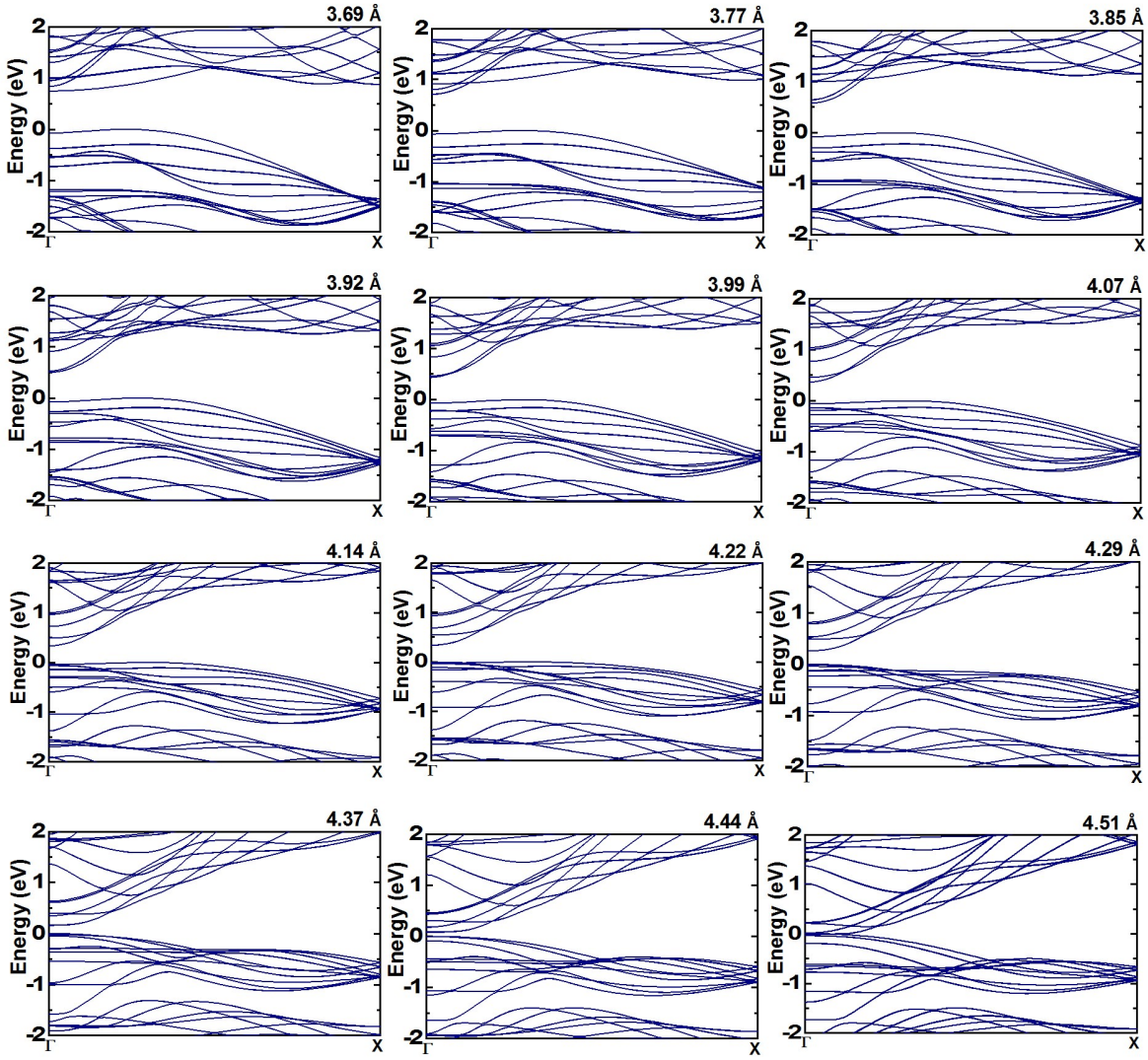

Fig. S4 Electronic band structure for the stretched (0, 9) nanotube.

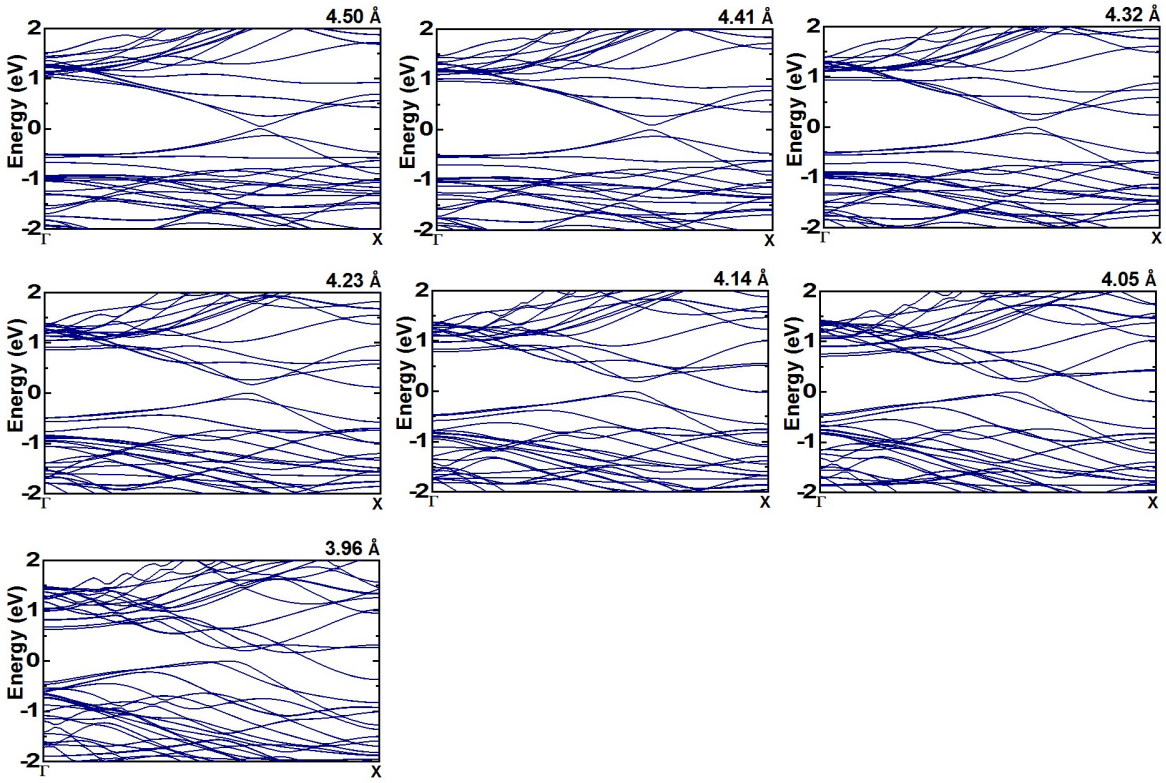

Fig. S5 Electronic band structure for the compressed (14, 0) nanotube.

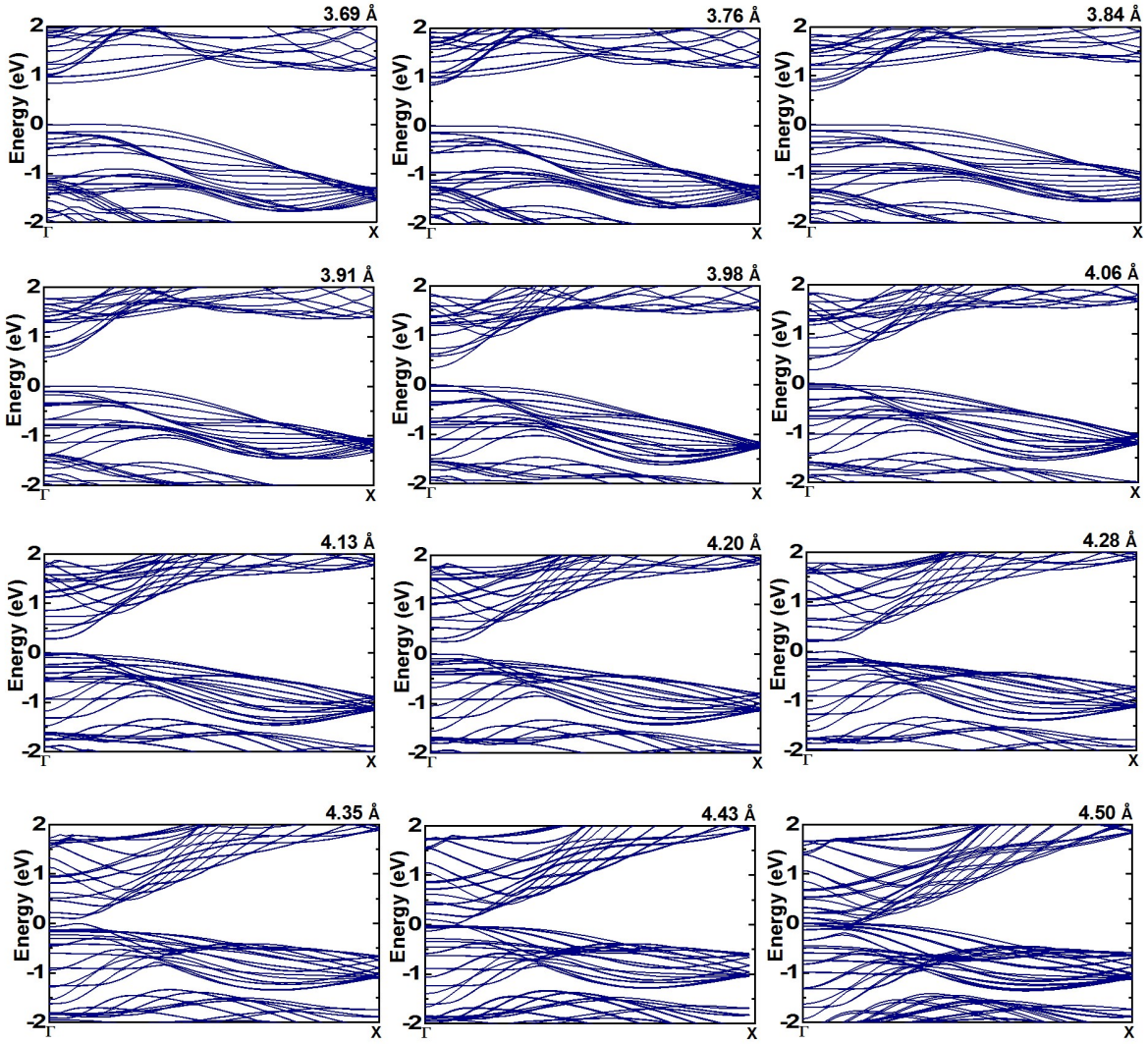

Fig. S6 Electronic band structure for the stretched (0, 14) nanotube.