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Tuning Circular Carbon Nanotubes into Regular Polygons via Selective Hydrogenation[1] GUANGFEN WU, Southeast University (China), University of Tennessee-Knoxville, JINLAN WANG, Southeast University (China), FENG DING, Hong Kong Polytechnic University — Using density functional theory approach, we study the selective hydrogenation of single walled carbon nanotubes (SWNTs). We confirmed that fully hydrogenated SWNT (FH-SWNT) is energetically more favorable than partially hydrogenated ones. Previous studies have revealed polygonization of bare carbon nanotubes (CNTs) through plasticity and buckling. Different from those traditional mechanical methods, we found that the curvature energy of a FH-SWNT can be significantly relaxed by the breaking of its cylindrical symmetry through a chemical pathway with low energetic compensation. Flipping a few rows of H over the FH-SWNT wall significantly reduces the tube curvature energy and leads to more stable configurations with polygonal (triangle, square etc) cross-sections.

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