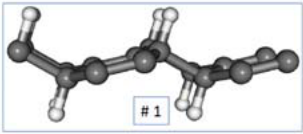
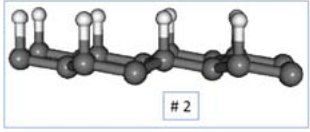
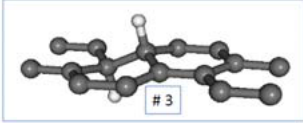
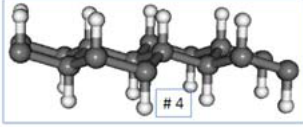
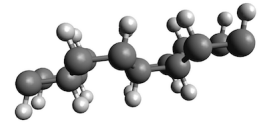


Graphane Data¹
 Sean Anderson & Reinaldo Zapata
 June 10, 2013

Name ²	Figure	Unit Cell	LDA Energy Gap (eV)	ecut (Ry) ³
C16H8 / C4H2 row close optimized translated to 16 8 / 50% H		Yes	3.58	45
C16H8 up / 16C 8H up / 50% H		Need	0.00	45
C16H2 / C16H2 row close 65Ry optimized / 12.5% H		Need	1.43 ⁴	65
Graphane Chair / C16H16 chair graphane / 100% H		Yes	3.12	65
Graphane Boat / 2x2 16C boat / 100% H		Yes	Need	65

¹All data from Phys. Status Solidi C 9, No. 6, 1378–1383 (2012) unless stated otherwise.

²Names include article reference, filename of XYZ file, and percent of H%

³Found in QE .in files.

⁴Data found on slide 6 of NANO_Bilayer_From OSI9_total_extra.pdf indicates that this is 1.2.