Supporting Information

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SI Text

Screw Dislocation Representation. Central to our discussion is a simple theorem, establishing the relationship between the arbitrary nanotube (n, m) and its equivalent representation as a *zigzag* tube with a screw *dislocation* along its axis:

$\forall(n, m)$, even $m \Leftrightarrow (n + m/2, 0)$ with dislocation of Burgers vector $\mathbf{b}_\gamma = m(-½, 1)$.

$\forall(n, m)$, odd $m \Leftrightarrow (n + m/2+½, 0)$ with $\mathbf{b}_\gamma = m(-½, 1)$ and an edge component $b_\perp = -½$.

Its validity can be seen by inspection of Fig. S1*A*. In the extreme case of an armchair tube, an example is shown in Fig. S1*B*.

Configurations for Energy Calculations. To determine the kink formation energy, the self-consistent DFT calculations were performed. While some details are discussed in *Methods*, calculations involve rather specific atomic configurations, which are shown here in Figs. S2 and S3. Results of the additional numerical tests, also discussed in *Methods*, are presented here in Table S1.

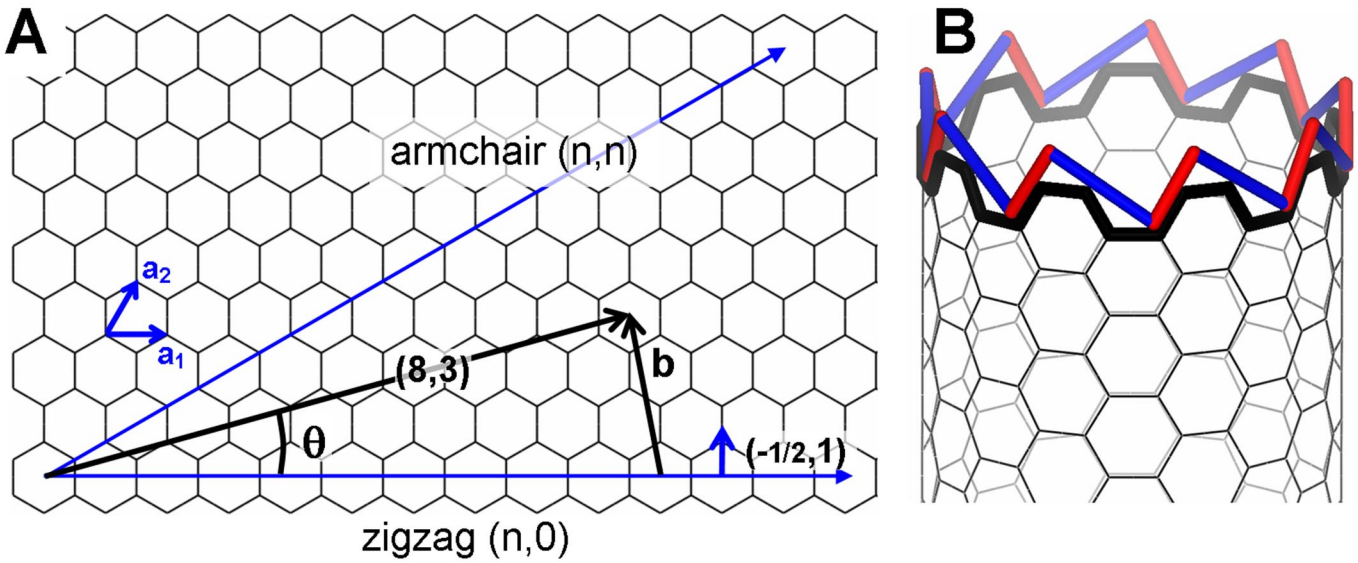

Fig. S1. (*A*) It is common to specify any nanotube by mapping its circumference vector onto a plane of hexagons, with the basis a_1 and a_2, so that the circumference vector is ($na_1 + ma_2$), or can be written as (*n*, *m*); chiral angle $0 < \theta < 30°$ is measured between the zigzag motif and the circumference, and, for the example shown here, the (8, 3) tube has a $\theta = 15.3°$. Alternatively, any single-walled carbon nanotube (n, m) can be viewed as a zigzag one, ($n + ½$m, 0) for an even m or ($n + ½m + ½$, 0) for an odd m, with a screw dislocation, $b_\gamma = m(-½, 1)$, and a small edge component $b_\perp = (-½, 0)$ for an odd *m*. The screw dislocation, $b_\gamma = m(-½, 1)$, corresponds to m kinks on the zigzag edge. (*B*) An (*m*, *m*) armchair tube can also formally be viewed as a zigzag (short blue zigzag segments) with m kinks (red); the example shown of a (9, 9) tube displays 9 sites where the new carbon can be added easily.

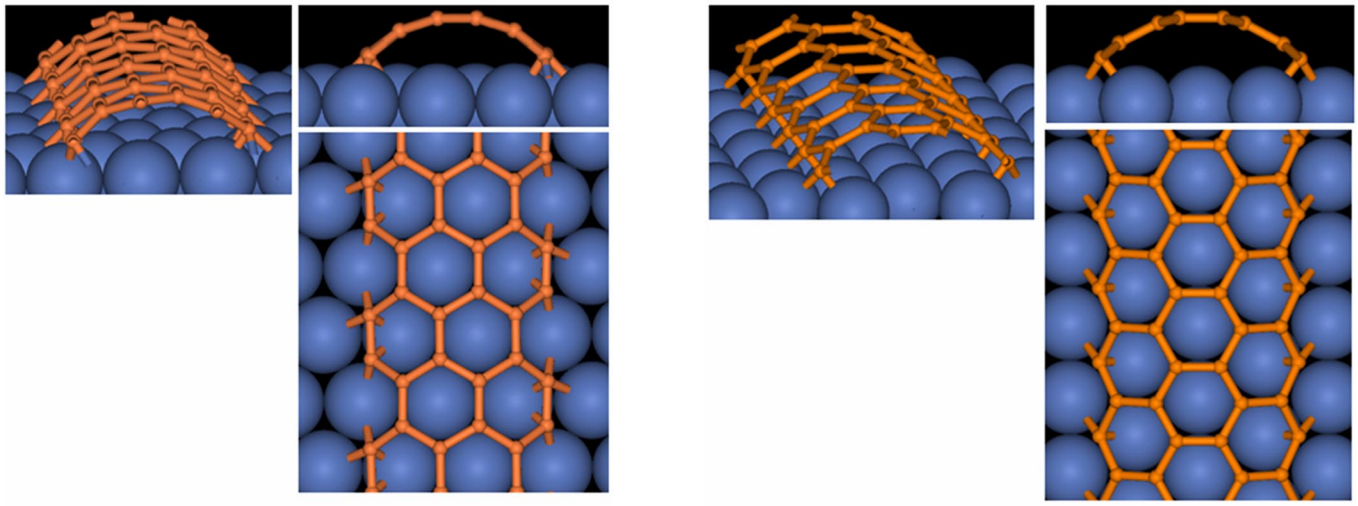

Fig. S2. Relaxed armchair and zigzag nanoribbon on an Ni (1, 1, 1) flat surface. (*Left*) Armchair strip/ribbon on an Ni (111) surface. (*Right*) Zigzag strip/ribbon on an Ni (111) surface.

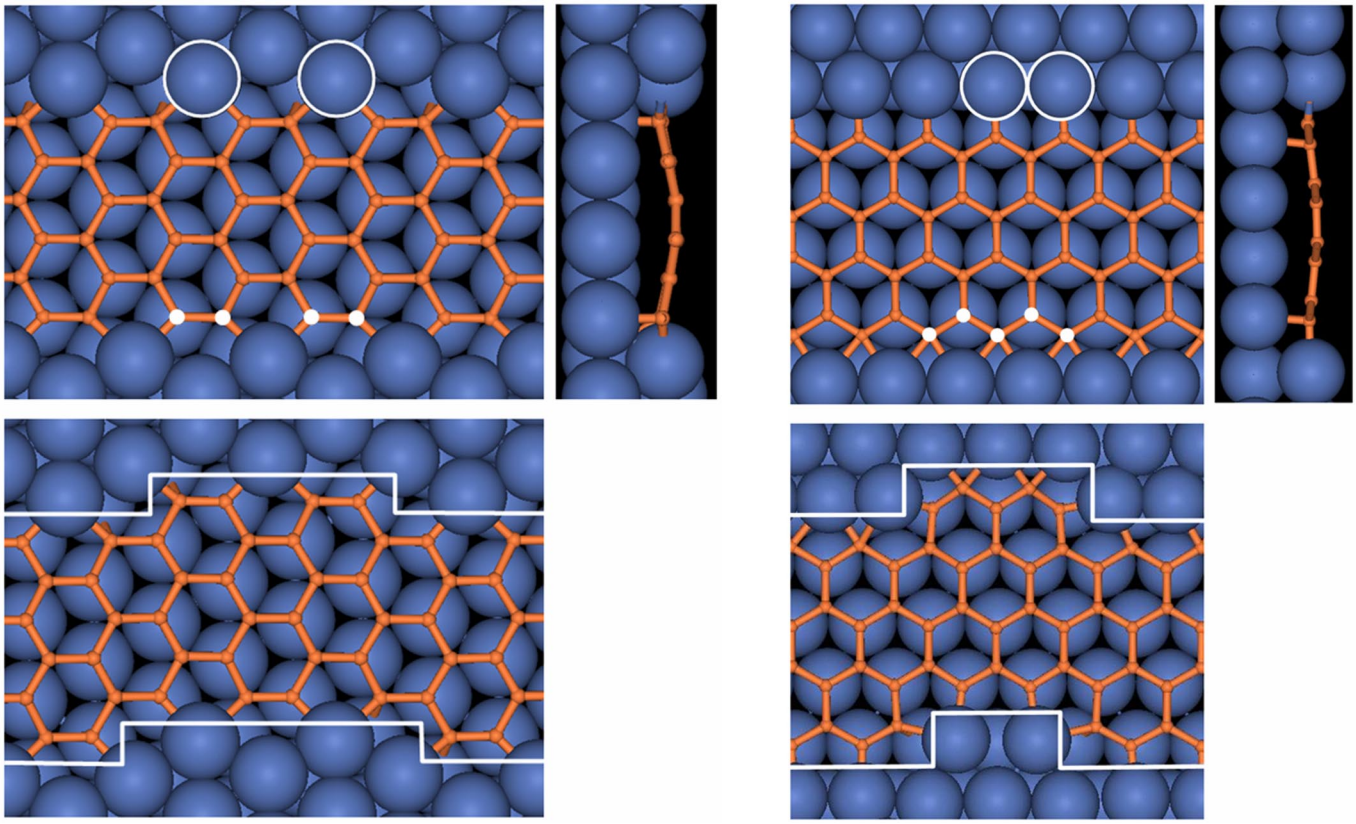

Fig. S3. Few C atoms (marked with white dots) are swapped with metal atoms (circled white) across the graphene strip/ribbon (*Top*), to create a quartet of kinks on the catalyst-graphene interface (*bottom*). *Left* shows the unit cell of an armchair ribbon located between the 2 metal steps and *Right* shows a unit cell for a zigzag case.

Table S1. Calculations for the C-contact with fully relaxed double layer of Ni

Contact	Energy calculated with gamma point (eV)	Energy calculated with 2x2x1 k-points (eV)
ZZ edge with kinks	−845.224	−845.288
ZZ edge without kinks	−847.949	−847.845
Nucleation barrier on ZZ edge	1.36	1.28
AC edge without kinks	−901.697	
AC edge with kinks	−901.635	
Nucleation barrier on AC edge	0.031	