

#### Electronic Supporting Information.

Detailed description of the **Movie S1**. A schematic show for the growth of a (4,2)  $\text{Au}_{0.5}\text{Ag}_{0.5}$ -NT in a confined (10,3) CNT at both the fixed (left) and unfixed (right) cases, obtained in our MD simulations. When the CNT is not fixed, the metal-metal atoms and carbon-carbon atoms interactions are described by the EAM and Tersoff potentials, respectively. And the metal-carbon interaction is described by the LJ potential. Our simulation result clearly shows that the inner (4,2)  $\text{Au}_{0.5}\text{Ag}_{0.5}$ -NT could still be formed in the MD simulation and outer (10, 3) SWCNT is not destroyed except that its diameter becomes a little bit larger at finite temperature. For example, the diameters of inner (4,2)  $\text{Au}_{0.5}\text{Ag}_{0.5}$ -NT and outside unfixed CNT reached 3.33 Å and 9.60 Å, respectively, in contrast to their previous values of 3.27 Å and 9.53 Å under the fixed CNT confinement. In a word, the condition of the fixed CNT would be appropriate for our MD simulations on the growth of transition metal alloy tubes in it.