The present talk will focus on the roles of nano-structured carbon materials in catalysis, including carbon nanotubes, graphene and heteroatom doped graphene. The emphasis is on some important energy conversion and chemical synthesis processes, i.e. the conversion of natural gas (methane) and syngas to the alternative energy such as liquid fuel and alcohols, as well as selective hydrogenation and selective oxidation of hydrocarbons. The nano-effects on catalysis such as the so-called size-dependency, quantum well states and synergetic confinement will be discussed through the examples. The unique effects of the electron confinement with CNT’s and the resulted modulating in catalysis will be illustrated. The techniques to introduce metal nanoparticles homogeneously inside the CNT channels have been developed and the effects of confined metal catalysts on their physio-chemical properties, as well as their catalytic activities have been studied systematically. Using Fe as a probe, it is found that the redox properties of metal oxide are modified when they are confined inside the CNT channels. In this way, a distinct enhancement of the CNT encapsulated Fe species to the F-T process and confined RhMn particles for the conversion of CO and H2 to ethanol have been achieved. Some of our recent results on the catalysis related to graphene materials will also be outlined in the talk.