The sharp rising of global energy demand is leading to continuous depletion of fossil fuels that has encouraged the development of renewable energy related technologies. The performances of these devices mostly depend on the materials used therein. Metal and carbon based nanomaterials are known to have efficient activities towards renewable energy harvesting, conversion and storage applications. In first part of this thesis, the development of catalysts for energy conversion reactions are discussed. Platinum based nanomaterials are promising to be used as electrodes in fuel cell, the most important green energy conversion device. However, their commercialization is limited by the high cost, poor efficiency and durability of the catalysts. Rare Pt morphologies such as tetrahedra, free-standing nanosheets, alloy nanowire membrane as well as biomass derived heteroatom doped carbon catalysts were synthesized, which has shown excellent activities and stabilities for fuel cell reactions compared to state of the art catalysts. The second part of this thesis is aimed to understand the self-assembly process of fullerene, an n-type semiconducting carbon allotrope, promising active component for solar energy harvesting as well as transistors, photo-detectors etc. Considering the importance of the self-assembly of C 60 by solution processing, which plays a crucial role in fabrication and thereby performance of these devices, the dependence of solvent shape and size on C 60 solvate formation was realized. Based on such understanding, a new C60 mediated isomer separation strategy was developed which resulted in 99.85% pure C8 (xylenes) and 99.95% pure C9 methyl substituted aromatic isomers, which are way above in purity over commercially available ones. Unique observations led us to develop single crystalline, oriented, free-standing C 60 films at ambient conditions by using water as liquid film-substrate, which is otherwise possible only with high vacuum system, can be useful for various device applications as well as fundamental studies.