In this talk, a brief overview of the roles of the quantum properties of nano-materials in new energy technology developments will be discussed. Some examples may include those in solar cells, fuel cells, catalysts, and artificial photosynthesis. I will highlight some key issues of the quantum physics researches and the contributions to energy technology developments. I will then discuss some results of our recent work on the first-principles understanding of the quantum properties of nano-materials for energy technology research. These include the quantum properties of nitrogen doped carbon nanotubes (CNTs) as new catalysts for dioxygen adsorption and reduction in hydrogen fuel cells. The aim of the work is to reduce the amount of the precious platinum (Pt) catalyst loading by identifying new catalysts for fuel cells. I will also discuss some results of our recent first-principles computations and experimental studies for the electronic properties of doped C60 fullerenes as new thermoelectric materials.