Study on the Electric-potential Properties of Nanotubes Using Computational Simulations

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In contemporary fuel cell technology, carbon-based nano-scaled materials display great potential to improve fuel efficiency and reduce cost. However, their relatively low activity limits the development and application of photovoltaic cells. In this study, capacitors and computationally constructed CNT(carbon nanotube) with MOFs(metal-organic frameworks) composites were studied to evaluate their thermodynamic and electrical efficiencies. To examine the efficiencies of the components used in current photovoltaic cells, possible nano-composites using computational analysis were constructed and tested for their efficacies. Both theoretical calculations for different geometries and computer simulations were performed to find the electrochemical properties in the nano-scaled materials. The stereo-chemical and thermo-dynamical properties were also found and analyzed.