

Panvika Pannopard 2014: Metal-decorated Carbon Nanotubes for Applications in Sensing and Catalysis: A Theoretical and Experimental Study. Doctor of Philosophy (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Professor Jumras Limtrakul, Ph.D. 180 pages.

The fabrication of metal nanoparticles decorated carbon nanotubes (MNPs-CNTs) is of current interest for the development of nanomaterial based catalysts and electronic devices. Here, the Density Functional Theory approach was employed to investigate the sensing and catalytic performances of MNPs-CNTs. The calculations show that Pt-doped CNT enhances, to a very large degree, the adsorptions and charge transfers of NO₂ and NH₃ toxic gas molecules and both processes cause changes in the electronic structure and charge distribution with greater and are more far-reaching than those of unmodified and defected CNTs. In the case of N₂O greenhouse gas decomposition, without metal doping, the reaction on the bare CNT proceeds via a high energy barrier (54.3 kcal mol⁻¹) which in the presence of active metals is reduced to 3.6, 8.0 and 10.2 kcal mol⁻¹ for V-, Ti- and Sc-doped CNTs, respectively. Thus, MNPs can overcome the limitations of intrinsic CNTs. For experimental work, the novel-designed catalytic platform for the fuel cell system was constructed whereby the Nafion layer and PtNPs were formed inside the pores of the CNT-Anodic Aluminium Oxide composite. The PtNPs are successfully deposited with chemical reduction and loading of the small size alkane-thiolated PtNPs. The thin layer of Nafion could also be coated properly to PtNPs size along the tube. Furthermore, the facile electrostatic deposition of the size-controlled AuNPs onto the negatively charged AAO-templated CNTs is demonstrated as a new strategy to produce the structure-controllable AuNPs/CNTs usefully for nanoapplications. By increasing the mole ratios of polyvinylpyrrolidone and dimethylaminopyridine (PVP:DMAP) stabilizers, the average diameters of AuNPs are progressively decreased. In addition, CNTs facilitate the Au depositions without tedious pretreatment on CNT surfaces.

Student's signature

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