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Generation of spinel $LiMn_2O_4$ nanotubes using computer simulation strategy

D M Tshwane, P E Ngoepe and **R R Maphanga**
University of Limpopo, South Africa

The importance of clean and efficient energy storage has grown enormously over the past decade, driven primarily by concerns of diminishing fossil-fuel reserves and increasing demand of portable electronic devices and grid storage systems. Nanotubes have drawn a continuous attention because of their unique electrical, optical and magnetic properties contrast to that of bulk system. They have potential application in the field of optical, electronics and energy storage device. Introducing nanotubes structures as electrode materials; represents one of the most attractive strategies that could dramatically enhance the battery performance. Spinel $LiMn_2O_4$ is the most promising cathode material for Li-ion batteries. In this work, computer simulation methods are used to generate and investigate properties of spinel $LiMn_2O_4$ nanotubes. Molecular dynamic simulation is used to probe the local structure of $LiMn_2O_4$ nanotubes and the effect of temperature on these systems. It is found that diameter, Miller indices and size have a direct control on nanotubes morphology. Furthermore, it is noted that stability depends on surface and wrapping of the nanotube. The nanotube structures are described using the radial distribution function and XRD patterns. There is a correlation between calculated XRD and experimentally reported results.

dmtshwane302@gmail.com

Effect of Gamma irradiation on the physical and chemical properties of copper/poly vinyl pyrolidone composite films

S A Waly, M M Shehata and **H H Mahmoud**
Nuclear Research Centre, Egypt

Polymer film based on poly (vinylpyrrolidone) (PVP) doped with different concentrations of copper nitrate were prepared using solution cast technique and the polymer films were subjected to 60Co γ-ray's source at various doses ranging between 100 and 400kGy. The effects of Cu ions concentration and gamma irradiation dose on the chemical and physical properties have been studied. The FT-IR spectra studies for undoped PVP and Cu/PVP films revealed the vibrational changes that occurred due to the effect of dopant copper in the polymer and gamma dose. The XRD results revealed that the amorphous domains of PVP polymer matrix increased in size with the increase of the doping concentration. The variation in film morphology was examined by scanning electron microscopy. Photoluminescence spectra were recorded for Cu/PVP films under the excitation wavelength of 750 nm and showed a decrease in luminescence intensity with increasing of the irradiation dose. The electrical conductivity increased with increasing of Cu dopant concentration and γ-irradiation dose. TGA and DTA studies reveal that changes in the thermal stability. Optical absorption studies were made in the wavelength range 200-800 nm. The absorption edge, direct and indirect band gap values were evaluated and the effect of gamma radiation on its value was determined. The direct band gap decreases from 3.4 to 3.09 eV and from 3.10 to 2.84eV for indirect band gap when the irradiation dose increases from 100kGy to 400kGy respectively.

shf_waly@yahoo.com