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Keywords: periodicity, nuclides, Farey-sequence

P11.05.128

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Preparation of cuprous oxide microspheres via HTAB-assisted glucose reduction approach

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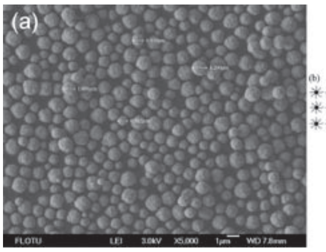
Cuprous oxide microspheres are widely used as catalysis, coatings, disinfection and anodic materials due to their unique assemble structures and their perfect dispersion and fluid properties. Cuprous oxide microspheres are usually fabricated by the thermal oxidation and the chemical vapor deposition which need high temperature or by the solution reduction which use the expensive or toxic materials as formaldehyde, sodium hypophosphite or KBH_4 as the reducing agents. Herein a moderate method was suggested to synthesis cuprous oxide microspheres via the hexadecyltrimethyl ammonium bromide (HTAB)-assisted glucose reduction approach, using $CuSO_4$ as the raw material. Dispersive uniform cuprous oxide microspheres (800-900nm) composed of crystalline nano-particles (8.5-13 nm) were synthesized by mixing $CuSO_4$ and glucose solutions in the presence of HTAB at room temperature followed by aging of the mixture at 70-80℃ for 0.5 h (Fig.1a). The presence of HTAB promoted the formation of cuprous oxide nano-particles as well as the subsequently assembly of the nano-particles to the cuprous oxide microspheres (Fig.1b).



Keywords: microspheres, cuprous oxide , glucose

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Crystal structures and high-temperature phase transition of Sr_2MSbO_6 (M=Sc,Cr,Fe) double perovskites

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The Sr_2MSbO_6 (M=Sc,Cr,Fe) materials have been elaborated by the standard solid state reaction method, and their structures studied with X-ray powder diffraction method, at room temperature (RT) and at high temperatures (HT). At RT, the crystal structures of these materials were found to have a monoclinic symmetry: Sr_2ScSbO_6, with $P2_1/n$ space group, and cell parameters a=5.6783(1), b=5.6923(1), c=8.0257(1) Å, β=89.98(1); Sr_2FeSbO_6, with $I2/m$ space group, and with a=5.6148(1), b=5.5954(4), c=7.9002(1) Å, β =90.02(4); and, finally, Sr_2CrSbO_6, with $I2/m$ space group, and cell parameters a= 5.5574(1), b= 5.5782(1), c= 7.8506 (1) Å, β=90.06(2). Depending on the M cation size, the M^{3+} and Sb^{5+} cations can be entirely or partially ordered, in the two distinct B-sites of the double perovskite structure. In the Sc compound, the Sc^{3+} and Sb^{5+} cations are totally ordered; in Cr and Fe, the M^{3+} (Cr^{3+},Fe^{3+}) and Sb^{5+} cations are partially ordered: the degree of the ordering is 99.4% and 92%, respectively. At HT, Sr_2ScSbO_6 undergoes three structural phase transitions: $P2_1$/n->I2/m->I4/m->Fm-3m, at about 400 K, 560 K and 650 K, which, to the best of our knowledgement, is the first time that such a rich phase-transition sequence has been observed in this kind of materials. Sr_2CrSbO_6 and Sr_2FeSbO_6 were found to present the I2/m->4/m->Fm-3m PT sequence: the first PT is discontinuous, and the second, continuous. In Sr_2CrSbO_6, the PT take place at about 500 and 660 K. In Sr_2FeSbO_6 the first PT starts to take place at 400 K, and shows a temperature interval, 400 to 420 K, in which both phases, monoclinic and tetragonal, co-exist; the second PT, from the tetragonal structure with $I4/m$ to the cubic structure with the Fm-3m, is observed above 500 K.

Keywords: transition-metal perovskites, powder diffraction method, phase transitions

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Powder structure determination of a series of homoleptic copper(I)-arylthiolate conducting polymers

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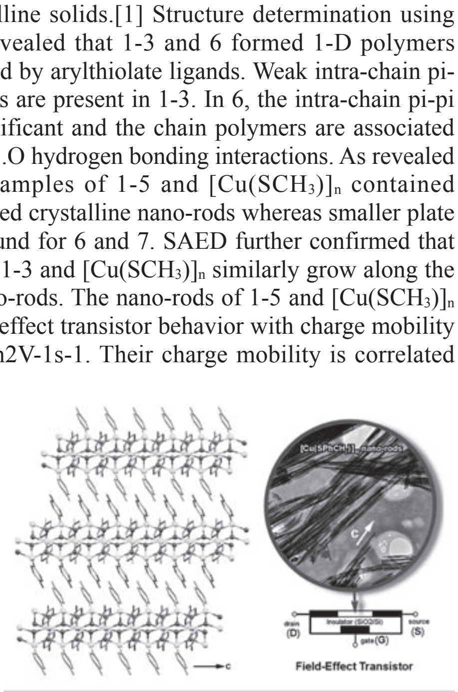
Homoleptic copper(I) arylthiolates $[Cu(p\text{-}SC_6H_4\text{-}X)]_n$ (X = CH_3 1, H 2, CH_3O 3, tBu 4, CF_3 5, NO_2 6, COOH 7 and n = infinity) were insoluble crystalline solids.[1] Structure determination using powder diffraction revealed that 1-3 and 6 formed 1-D polymers with Cu atoms bridged by arylthiolate ligands. Weak intra-chain pi-pi stacking interactions are present in 1-3. In 6, the intra-chain pi-pi interactions are insignificant and the chain polymers are associated via non-covalent C-H...O hydrogen bonding interactions. As revealed by TEM, the solid samples of 1-5 and $[Cu(SCH_3)]_n$ contained homogenously dispersed crystalline nano-rods whereas smaller plate nano-crystals were found for 6 and 7. SAED further confirmed that the chain polymers of 1-3 and $[Cu(SCH_3)]_n$ similarly grow along the long axes of their nano-rods. The nano-rods of 1-5 and $[Cu(SCH_3)]_n$ exhibited p-type field-effect transistor behavior with charge mobility of 10E-2 to 10E-5 cm2V-1s-1. Their charge mobility is correlated to their unique chain-like copper-sulfur networks, and the para-substitutent of arylthiolate ligand alter the ultimate particle morphology and charge transport properties.



$[Cu(SPhCH_3)]_\infty$ nano-rod FET device

[1] Chem. Eur. J. 2008, 14, 2965.

Keywords: *ab initio* powder structure determination,