Abstract

The new layered niobate Cu0.5Nb3O8 is synthesized by soft chemistry in aqueous electrolyte via $Cu^{2+} \rightarrow H^{+}$ exchange between copper nitrate and HNb3O8·H2O. The characterization of the exchanged product is made by means of thermal gravimetry, chemical analysis, X-ray diffraction and IR spectroscopy. Thermal analysis shows a conversion to anhydrous compound above 500°C. The oxide displays a semiconductor like behavior; the thermal variation of the conductivity shows that d electrons are strongly localized and the conduction is thermally activated with activation energy of 0.13 eV. The temperature dependence of the thermopower is indicative of an extrinsic conductivity; the electrons are dominant carriers in conformity with an anodic photocurrent. Indeed, the Mott-Schottky plot confirms n-type conduction from which a flat band potential of -0.82 VSCE, an electronic density of 8.72×10^{19} $m^{-3}$and a depletion width of 4.4 nm are determined. The upper valence band, located at ~5.8 eV below vacuum is made up predominantly of Cu^{2+}: 3d with a small admixture of O^{2-}: 2p orbitals whereas the conduction band consists of empty Nb^{5+}: 5s level. The energy band diagram shows the feasibility of the oxide for the photocatalytic hydrogen production upon visible light (29 mW cm^{-2}) with a rate evolution of 0.31 mL g^{-1} min^{-1}