



# Electronic structure, growth and properties of hydrothermally derived crystalline $\text{Cu}_2\text{MnSnS}_4$ quantum dots: optimization of physiochemical parameters and electrochemical performance

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## Abstract

The present article reports the synthesis, characterization and spin-polarized electronic structure of  $\text{Cu}_2\text{MnSnS}_4$  (CMTS) quantum dots. Optimization of the hydrothermal physical parameters including reaction temperature and duration has been performed. The CMTS material synthesized was characterized for its structural, morphological, chemical, compositional optical and electrochemical properties. Variation of the reaction parameters made it possible to get an idea about the process of material formation. Formation mechanism, secondary phase detection and single-phase crystallinity are achieved robustly. Single phase tetragonal CMTS was synthesized just after 8 h reaction duration. Significant reactions parameters like, prolonged reaction duration and higher temperatures influence the morphology and hence resulted in enhanced crystallinity of these nanostructures. Variable structural morphologies and shapes like polygons, cauliflower and quantum dots as small as 4–5 nm were synthesized. Optical properties indicated that the quantum dots are highly active in the visible range of the optical spectrum. Also, the electronic structure calculations for this material tracked the 1.4 eV band gap confirmed from absorption spectrum. Electrochemical properties showed the material is having pseudocapacitive nature exhibiting specific capacitance of 268 F/g revealing its charge storing ability.

**Keywords** CMTS · Quantum dots · Electronic structure · Pseudocapacitance · Charge storing

## 1 Introduction

Eco-friendly and proficient energy storage systems are very significant to fulfill the growing demands. Supercapacitors are playing a leading role as energy storage systems.

Because of small mass, high compactness and prompt charge–discharge ability, supercapacitors (SCs) serve as important energy storage systems [1, 2]. Metal oxides, sulphides and hydroxides are used as electrode materials in pseudocapacitors, while graphene, carbon nanotubes, activated carbon and carbon-aero gels are used in electric double layer capacitance (EDLC) [3, 4]. Chalcogenide nanostructures have shown great ability in charge storing. Quaternary chalcogenide semiconductors based on earth-abundant elements,  $\text{Cu}_2\text{XSnS}_4$  ( $X = \text{Mn, Zn, Co, etc.}$ ) have been materials of great attention due to their multiple applications like in thermoelectrics, Photocatalysis, gas sensing, supercapacitors, etc. Copper-based quaternary chalcogenides inherit certain properties such as optimum bandgap (1.0–1.5 eV), high absorption coefficient, that make these materials suitable for solar cells and supercapacitors [5]. CMTS belong to the metal chalcogenide family comprising of earth abundant elements. There are various reports on the chemical synthesis of CMTS nanostructures [6]. CMTS has being explored for various applications including solar cells, photocatalysis,

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