



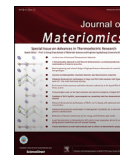
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Layered oxychalcogenides: Structural chemistry and thermoelectric properties

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Abstract

Layered oxychalcogenides have recently emerged as promising thermoelectric materials. The alternation of ionic oxide and covalent chalcogenide layers found in these materials often results in interesting electronic properties, and also facilitates the tuning of their properties via chemical substitution at both types of layers. This review highlights some common structure types found for layered oxychalcogenides and their interrelationships. This review pays special attention to the potential of these materials for thermoelectric applications, and provides an overview of the thermoelectric properties of materials of current interest, including BiCuSeO.

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Keywords: Oxychalcogenides; Layered structures; Thermoelectric; BiCuSeO

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1. Introduction

Layered oxychalcogenides are mixed-anion compounds, in which oxide and chalcogenide anions (Group 16) indirectly bound via one or more cations, creating a stack of alternating oxide and chalcogenide layers. The coexistence of ionic oxide anions and more covalent chalcogenide anions leads to a highly distinctive structural chemistry. Owing to the preference of “hard” non-polarisable cations to coordinate to smaller oxide anions, while “soft” more polarisable cations preferentially coordinate to larger chalcogenide anions, quaternary oxychalcogenides tend to adopt structures in which oxide and chalcogenide anions are segregated, with each coordinating preferentially to one type of cation, as early noted by Guittard et al. [1]. This often results in structures with low-dimensional characteristics, and structural low dimensionality may lead to highly anisotropic electronic band structures, together with interesting electronic properties. In addition, the covalent character of the chalcogenide layers promotes high-mobility semiconduction, whereas low thermal conductivity is favoured by the more ionic interactions of the oxide blocks. The alternation of distinct layers found in oxychalcogenides also facilitates the tuning of their properties via chemical substitution at both the oxide and chalcogenide layers. The coexistence of low-dimensionality together with covalent and ionic bonding offers great potential for thermoelectric applications, and can also result in a wide range of unexpected and fascinating properties. For instance, $\text{Ce}_2\text{O}_2\text{S}$ nanoparticles anchored on graphitised carbon has been recently found to be a promising

anode material for Li-ion batteries, with a stable specific capacity up to 627 mA h g^{-1} after 180 charge–recharge cycles [2]. $\text{Sm}_2\text{Ti}_2\text{S}_2\text{O}_5$ has attracted considerable attention as a photocatalyst for water splitting [3], and LaOCuS is considered a promising *p*-type transparent semiconductor for optoelectronic applications [4]. Superconductivity has been recently reported in bismuth oxysulfides, although the T_c is rather low $\sim 4.5 \text{ K}$ [5–7]. An improvement of the superconducting properties of compounds containing $[\text{BiS}_2]^{2-}$ layers has been found in electron doped $\text{NdO}_{0.5}\text{F}_{0.5}\text{BiS}_2$ ($T_c \sim 5 \text{ K}$) [8] or $\text{LaO}_{1-x}\text{F}_x\text{BiS}_2$ ($T_c \sim 10.6 \text{ K}$) [9].


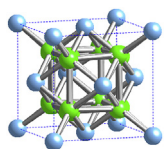


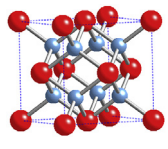
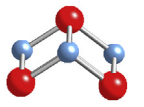

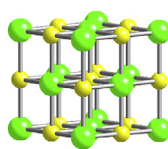
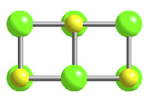

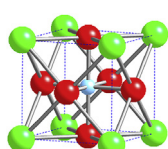
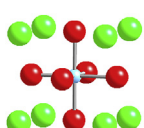
Although oxychalcogenides can also adopt structures without low-dimensional characteristics, as exemplified by $\text{Eu}_5\text{V}_3\text{S}_6\text{O}_7$ and $\text{La}_{10}\text{Se}_{14}\text{O}$ [10], throughout this review we restrict our scope to layered oxychalcogenides, with a particular focus on their potential for thermoelectric applications. The structures of some families of layered oxychalcogenides have been previously reviewed [1,11,12].

2. Structural chemistry of layered oxychalcogenides

2.1. Common building blocks

Structures of layered oxychalcogenides can be described as a combination of two (or more) types of building blocks. Certain inorganic slabs, such as perovskite, fluorite, or rock-salt blocks, which are encountered in many structures, can be considered as two-dimensional building blocks, and layered structures in which two or more types of such building blocks

Table 1
Common building blocks found in oxychalcogenides.

Structure	Unit cell	Building block slab	Key
Fluorite (CaF_2) 			Ca^{2+} (blue) F^- (green)
Antifluorite (Na_2O) 			Na^+ (blue) O^{2-} (red)
Rock-salt (NaCl) 			Na^+ (yellow) Cl^- (green)
Perovskite (SrTiO_3) 			Sr^{2+} (green) Ti^{4+} (blue) O^{2-} (red)

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