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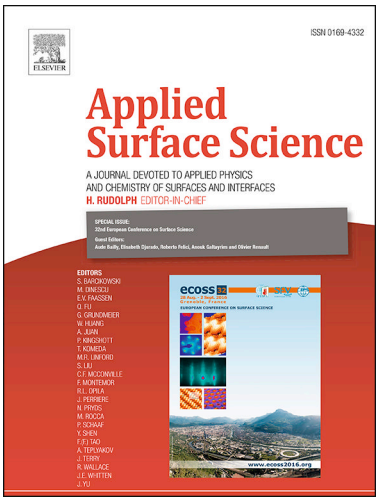

Full Length Article

Geometry, electronic structure, morphology, and photoluminescence emissions of $BaW_{1-x}Mo_xO_4$ (x=0, 0.25, 0.50, 0.75, and 1) solid solutions: theory and experiment in concert

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Geometry, electronic structure, morphology, and photoluminescence emissions of $BaW_{1-x}Mo_xO_4$ (x=0, 0.25, 0.50, 0.75, and 1) solid solutions: theory and experiment in concert

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Abstract

The design of a solid solution with tunable electro-optical properties and multifunctionality is a promising strategy for developing novel materials. In this work, $BaW_{1-x}Mo_xO_4$ (x=0, 0.25, 0.5, 0.75, and 1) solid solutions have been successfully prepared for the first time by a co-precipitation method. Their crystal structure and phase composition were determined by X-ray diffraction and Rietveld refinements. Fourier transform infrared and micro Raman spectroscopy in combination with field-emission scanning electron microscopy (FE-SEM) were used to describe the microstructures and chemical compositions of the synthesized materials. The influence of chemical composition on morphology and photoluminescence (PL) emission has been analyzed. The geometry, electronic structures, and morphologies of $BaW_{1-x}Mo_xO_4$ (x=0, 0.25, 0.5, 0.75, and 1) solid solutions were investigated by first-principles quantum-mechanical calculations based on the density functional theory. By using Wulff construction and the values of the surface energies for the (112), (001), (110), (101), (100), and (111) crystal faces, a complete map of the available morphologies for the $BaW_{1-x}Mo_xO_4$ solid solutions was obtained. These results show a qualitative agreement between the experimental morphologies obtained using the FE-SEM images and the computational models. The substitution of W^{6+} by Mo^{6+} enhances the electron-transfer process due to a stronger Mo(4d)-O(2p) hybridization compared to W(5d)-O(2p) for the W/Mo-O superficial bonds, and is responsible for the change in morphology from $BaWO_4$ to $BaMoO_4$. Such a fundamental study, which combines multiple experimental methods and first-principles calculations, has provided valuable insight into obtaining a basic understanding of the local structures, bonding, morphologies, band gaps, and electronic and optical properties of the $BaW_{1-x}Mo_xO_4$ (x=0, 0.25, 0.5, 0.75, and 1) solid solutions.

1. Introduction

Alkaline earth molybdate and tungstate ($AMoO_4$ and AWO_4, A = Ba, Sr, or Ca) are inorganic compounds having the scheelite-type ABO_4 structure, and exhibit interesting properties for a wide range of applications such as

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