Electronic Structure Investigations of Several Orthovanadates

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Orthovanadates (AVO_4, where A is a trivalent element) have recently emerged as promising optical materials for birefringent solid-state laser applications[1,2]. They can be also employed in a number of applications including their use as cathodoluminescent materials, thermophosphors, and scintillators[3]. We considered several systems with A= Sc, Y, La, Eu, Gd, and Lu. To give insight into electronic structures of the systems we employed the full potential local orbital (FPLO[4]) method. We'll present the band structure, local and total densities of electronic states. For the Eu and Gd systems the magnetic moments will be presented. The calculations showed that the band gap in electronic spectrum depends on A element and varies from 0 to 3.28 eV.

References:

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