First-principles calculations of YPO_4, YVO_4, $YNbO_4$ and $YTaO_4$: Electronic structures and Luminescent properties

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1. Introduction

The nature of optical excitations near the band gap of YPO_4, YVO_4, $YNbO_4$ and $YTaO_4$ is studied using first-principles band structure methods. It is shown that absorption near the band edge in YRO_4 (R = P, V, Nb and Ta) involves excitations from the oxygen 2p-like bonding states near the top of the valence band (VB) anti-bonding states to the cations *n*d-like near the bottom of the conduction band (CB).

2. Methodology

We have performed first-principles electron densities of states (DOS) calculations based on the density functional theory. Single point DFT calculations were carried out as implemented in the $DMol^3$ program package of Molecular Simulation Inc.. We have taken a non-local density approximation, so-called the generalized gradient approximation (GGA) functional suggested by Perdew and Wang. As the basis sets, we have used double numerical basis functions with polarization functions (DNP) for all the calculations. The relativistic effective core potential (ECP) approximation was used for the core electrons of Y, V, Nb and Ta. All calculations were carried out in the spin-restricted model.

3. Results

We found that the calculated energy gaps from band calculations for YRO_4 (R = P, V, Nb and Ta) agree with the observed gap of 3.9 ~ 5.6 eV. The band gap of YPO_4 consists of O 2p-like states and Y 4d-like states. Minor variations of the band gap among YVO_4, $YNbO_4$ and $YTaO_4$ are possibly due to variations in their crystal structures and the relative ordering of 5th ionization potential energy of V, Nb and Ta.