Interrelationships between the luminescent transitions and nonlinear optics in RE activated phosphate, arsenide and vanadate compounds

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We discuss the influence of orbital hybridization on the intensity of the hypersensitive transition in isostructural vanadate arsenide and phosphate systems. We found out that the same mechanism is also responsible for the efficiency of second harmonic generation (SHG). Second harmonic generation (SHG) is a nonlinear process in which a crystal converts lower frequency radiation to higher frequency. The bonding covalence within the acentric anionic groups, that are the basic structural moiety of the crystal framework (such as PO_4, AsO_4, VO_4, SiO_4, GeO_4, etc.), is chiefly responsible for the SHG activity. The importance of orbital hybridization on the SHG efficiency is exemplified by the striking difference in optical nonlinearity between isostructural titled compounds. While the vanadate is efficient, the phosphate shows no SHG activity, although the calculated SHG coefficients (pm/V) for both compounds are non-zero. The difference in the SHG efficiency has been clarified by examining the electronic band structure of these compounds. Our analysis supports the polarizability of $(XO_4)_3$- (X = P, As, V) over local site distortion effects as the intensity enhancing mechanism of the $^5D_0 \rightarrow ^7F_2$ transition. The connection between the mechanism of hypersensitivity and second harmonic generation (SHG) is presented.

[1] A M Srivastava, M G Brik, W W Beers, Chong-Geng Ma, M Piasecki, W E Cohen (2023) J.Lumin. 257, 119709.
[2] A. M. Srivastava , M G Brik, B. Lou, W W Beers, Chong-Geng Ma, M Piasecki, W E Cohen (2023) ECS J. Solid State Sci. Technol. 12 066001

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