First-Principles Study on Electronic Structures and Optical Properties in the Zinc Pyrovanadates Using Quasi-Particle Self-Consistent GW Method

Selim Reza

Graduate School of Natural Science and Technology, Kanazawa University, Japan

Masao Obata

Graduate School of Natural Science and Technology, Kanazawa University, Japan

Tatsuki Oda

Graduate School of Natural Science and Technology, Kanazawa University, Japan

Abstract:

First-principle investigations of the structural, electronic and optical properties of the low- and high-temperature phases of zinc pyrovanadate were analyzed using density functional theory (DFT) and quasi-particle self-consistent GW approximations (QSGW). The computed structures have a potential applications in energy storage (supercapacitors, batteries, hydrogen storage) and catalysis. We report results computed with QSGW approach for the first time for the material under consideration, along with a comparison with DFT. The structural aspects for both phases are discussed at a greater length, mentioning the noticeable differences. The total energies obtained from GGA-PBE shows more stability for low-temperature phase (α phase) than for the high-temperature (β phase) phase which is consistent with experimental findings. The calculations of electronic band structure for the both phases indicates indirect semi-conducting nature with wide band gap value. The GGA-PBE computation provides underestimated band gap as usual while QSGW calculations largely overestimate. The band structure also reveals that the β phase is more disperse than the α phase, owing to the high symmetric position due to increasing temperature. The density of state calculations display the differences between the phases that arises from the structure. Moving of bridging oxygen between two vanadium atoms towards a higher symmetric and more hybridized position with vanadium atom resulting in changing the space group from *C2/c* to *C2/m*. The crystal field effect (splitting of *d* orbital) is studied for *V-3d* orbital due to negative charges of tetrahedrally coordinated oxygen atoms. The optical property calculations suggest some potential applications for the optoelectronic devices.

Keywords:

Ab-initio calculations, Density functional theory, GW approximations, Structural study, Electronic study, Optical properties.