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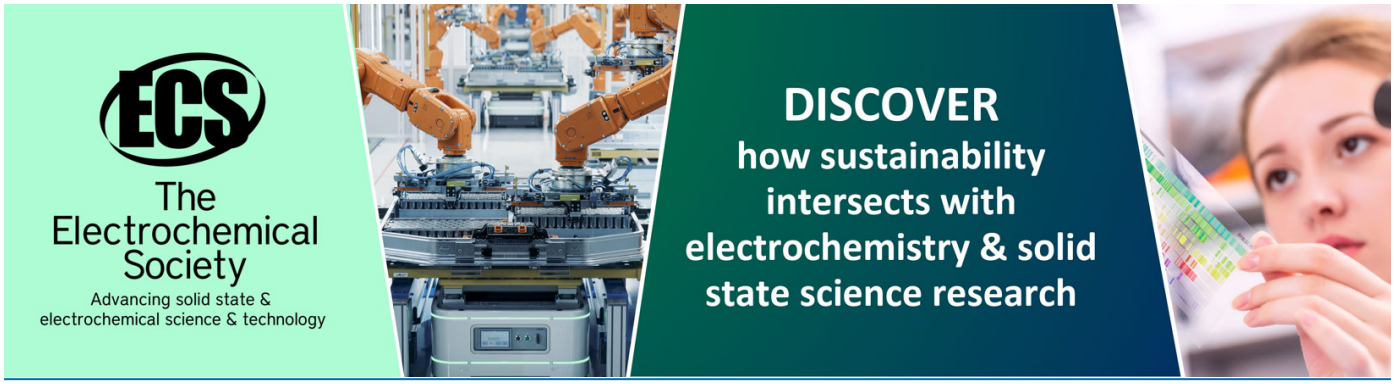

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The Band Structure of a Rare Earth Element of Promethium (III) Oxide (Pm_2O_3) Calculated Using Density Functional Theory

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Abstract. Luminescence is emission of light by a substance not resulting from heat. It is form of cold body radiation. It can be caused by chemical reactions of the substance with other substances around it, electrical energy, subatomic motions or stress on a crystal. There are many types of luminescence. One of it is phosphorescent. Phosphorescent is made from phosphors such as doped strontium aluminate. Phosphorescent emission light persists long after it has been exposed to light and will fading over time. Promethium (Pm) is low energy beta emitter. It does not degrade the phosphor lattice and the luminosity of the material does not degrade so fast. Promethium based paints are safer than Radium (Ra) and have half-life about more than two years. Promethium usually found in form oxidation called promethium (III) oxide (Pm2O3) and usually applied on watch and phones dial. The study of a band structure of Pm2O3 has not been covered yet. By using density functional theory, we calculated the band gap of promethium (III) oxide from it crystalline structure. The calculated band structure show a clear band gap between valence and conduction band at Fermi level. However the value shows very small gap at 0.286 eV. The density of state and partial density of states has been produced. The calculation has been done using different type of approximation from general gradient approximation (GGA).

1. Introduction

Luminescence is emission of light by a substance that not resulting from heat. This is form of cold body radiation. Luminescence usually caused by chemical reactions, electrical reactions, subatomic motions, or stress on a crystal. This distinguishes luminescence from incandescence [1]. As we know, incandescence is light emitted by a substance that resulted from heating. Nowadays, the dials, hands and scales and navigational instruments and markings are often coated with luminescent materials. There are many types of luminescence such as fluorescence, phosphorescence, and radioluminescence.

Fluorescence is the emission of light by a substance that has absorbed light or electromagnetic radiation. While, phosphorescence is mechanism for producing light similar to fluorescence, but the emission of visible light persists long after it has been exposed to the light. One of materials emitting this type of luminescence is phosphors. Phosphor can absorb energy from the incident radiation that fall onto it and emit photons [1]. Radioluminescence is the phenomenon by which light is produced by materials by bombardment with ionizing radiation, such as beta particles. It contains a radioactive isotope that combined with radioluminescence substance. Radioactive materials that usually used in radioluminescence type of emission are radium (Ra), tritium (3H) and promethium (Pm) [3].

Promethium element is relatively low-energy beta-emitter, which unlike alpha emitters, does not degrade the phosphor lattice and the luminosity and does not degrade so fast. Furthermore, promethium is quite safer than radium.

Usually, rare earth elements are ideal elements for spectral conversion because of their high luminescence characteristics. Rare earth elements rich with energy level structure that allows for great flexibility on conversion of photons in wide spectral region [1]. Promethium is one of the rare earth materials, but usually it is form by bombardment of uranium-235 and thermal neutrons.

Promethium is one of the radioactive substances in the lanthanide group [3,4]. Promethium can be prepared artificially in particle accelerators or known as “atom smashers”. All of promethium isotopes elements are known are radioactive. The common form of promethium is promethium (III) oxide. Recently, lanthanide group of elements have been doped into wide band gap semiconductor to produce light in different range of wavelength especially at visible light range and UV spectrum at different temperature [5].

Density functional theory (DFT) has been used to simulate the structure of material at the ground state energy to calculate the density of state, energy gap and produce a band structure. The exchange-correlation potential in the Kohn-Sham equation can be solved using local density approximation (LDA), generalized gradient approximation (GGA) and hybrid [6,7,8]. No calculation has been publish on promethium using DFT or other calculation method. In this paper, we calculate the density of state, band gap structure and measure the band gap of promethium (III) oxide with different type of GGA approximation. Previously, we have done a calculation on several types of oxide material and agreed with the experimental result. We also measured the band gap of abundant material using GGA, however it shows small shift when comparing with an experimental result.

2. Material and method

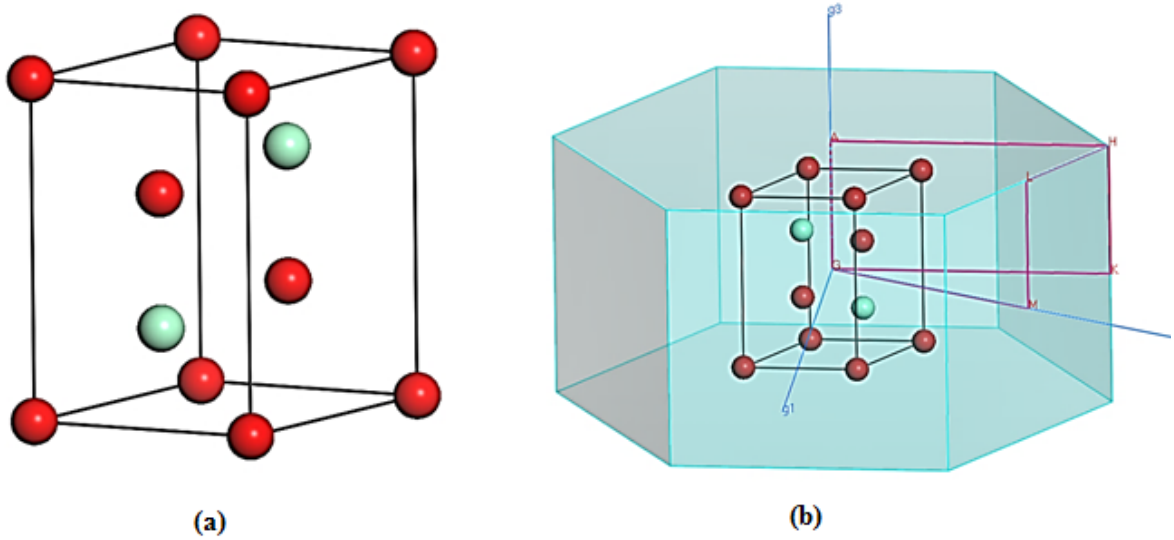

Figure 1: (a) Structure of promethium (III) oxide and (b) Brillouin zone of promethium (III) oxide using CASTEP module.

We are using the density functional theory (DFT) calculation in CASTEP software. There are many approximation can be used in CASTEP software such as local density approximation (LDA), generalized gradient approximation (GGA) and Heyd-Scuseria-Ernzerhof (HSE). The scope of this analysis focused on the band gap and density of states (DOS) of the structure promethium (III) oxide

using GGA with different exchange-correlation functional such as Perdew-Burke-Ernzel (PBE), Perdew-Wang 91 (PW91), revised Perdew-Burke-Ernzerhof (RPBE) and Perdew-Burke-Ernzerhof revised for solids (PBESOL). DFT is a predictive calculation and very accurate almost for material with low percentage error [6,7,8].

3. Result and discussion

The calculation has been done using GGA PBESOL, PW91,PBE and RPBE. It show that RPBE has a higher band gap for Pm_2O_3 as shown at table 1. However, this calculation is far from the hybrid method as well as Hubbard-U model.

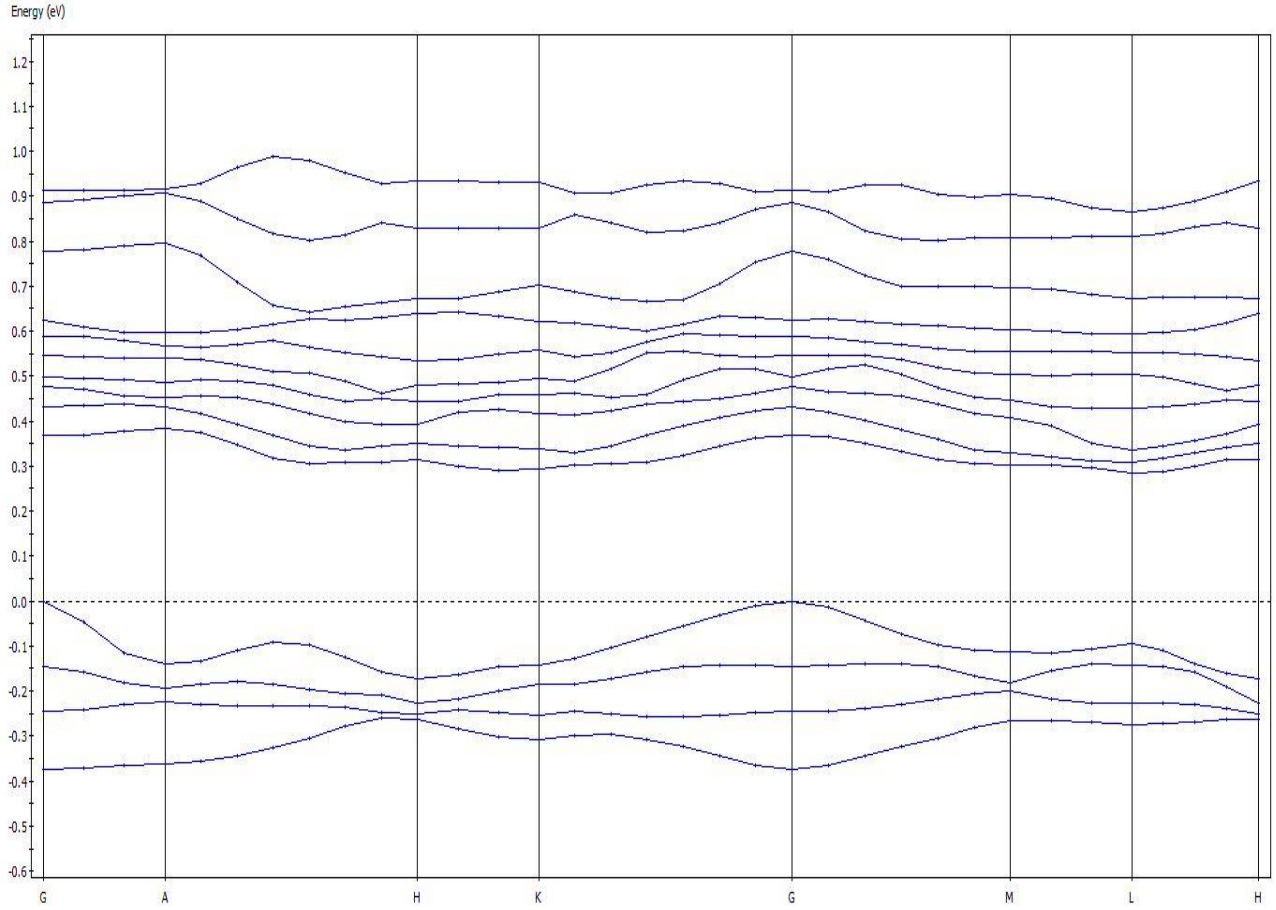

Figure 2: The band structure of Pm_2O_3 calculated using PBESOL approximation of GGA.

Table 1: The value of band gap energy in promethium (III) oxide with different exchange correlation functional of GGA

Exchange correlation functional of GGA	PBESOL	PW91	PBE	RPBE
Band gap (eV)	0.286	0.707	0.790	0.991

4. Conclusion

We able to obtained the band gap of promethium (III) oxide using different approximation of exchange-correlation, but it is very small compared to other research that uses hybrid functional which is within 4.8 to 5.6 eV [2]. The band gap energies obtained is very small in range 0.2~1.0 eV.

References

[1] Kabongo, G. L., Luminescence investigation of zinc oxide nanoparticles doped with rare earth ions. (2013) MSc dissertation. University of South Africa

[2] Gillen, R., Clark, S. J., & Robertson, J., Nature of the electronic band gap in lanthanide oxides. *Physical Review B*, *87*(12), (2013). 125116.

[3] Voncken, J. H. L., The Rare Earth Elements—A Special Group of Metals. in The Rare Earth Element*s,* Springer International Publishing, (2016) 1-13.

[4] Azimi, G., Dhiman, R., Kwon, H. M., Paxson, A. T., & Varanasi, K. K., Hydrophobicity of rare-earth oxide ceramics. *Nature materials*, *12*(4), (2013) 315-320.

[5] Birkhahn, R. H., Chao, L. C., Garter, M. J., Scofield, J. D., & Steckl, A. J., *U.S. Patent No. 6,255,669* (2001).

[6] W. Kohn, Nobel Lecture: Electronic structure of matter-wave functions and density functionals. *Rev. Mod. Phys.* 71(5), (1999) 1253-1266.

[7] W. Kohn & L. J. Sham, Self-Consistent Equations Including Exchange and Correlation Effects. *Phys. Rev.* 140, (1965) A 1133 – A 1138.

[8] P. Hohenberg & W. Kohn, Inhomogeneous Electron Gas. *Phys. Rev.* 136, (1964) B864 – B871.

[9] Basri, Katrul Nadia; Zabidi, Noriza Ahmad; Abu Kassim, Hasan; Rosli, Ahmad Nazrul (2015). Density Functional Theory (DFT) Calculation of Band Structure of Kesterite, Advanced Materials Research, 1107, 491-495.