National Conference on Computational Composite: Power of Synthia 15-17 Nov 2020

Prediction of Optical, electrical and thermal properties for a composite of bisphen dimeth carbonate and benz imidazoles

Truptimayee Rath¹, Mr. Chittaranjan Routray²

¹180705100086@cutm.ac.in, ²chittaranjan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: A computational study has been done to predict Optical, electrical and thermal properties of a polymer composite consisting of bisphen_dimeth_carbonate and benz_imidazoles. Synthia module of Biovia Materials Studio software was used to predict Refractive index, Volume resistivity, Dielectric constant, Coefficient of volumetric thermal expansion and Thermal conductivity of the composite.

Objective: In this study the effect of mixing of bisphen_dimeth_carbonate and benz_imidazoles on the following properties have been predicted.

- a. Refractive index
- b. Volume resistivity
- c. Dielectric constant
- d. Coefficient of volumetric thermal expansion
- e. Thermal conductivity

The weight fractions of the monomers were varied in the range of 0 to 1.

Software used: Synthia module of Biovia Materials Studio software (Dassault Systemes, France) was used for the study.

Results and Discussion: The effect of weight fraction of bisphen_dimeth_carbonate (Monomer 1) on the Optical, electrical and thermal properties of the composite has been presented in Table 1. The predicted properties of the composite for 0, 0.5 and 1.0 weight fractions of bisphen_dimeth_carbonate have been summarized in Table 1. The rate of change for the properties have been summarized in Table 2.

Table 1. Properties of composite of bisphen dimeth carbonate and benz imidazoles

Property		Results for		
Name	Unit	0.0 weight fraction of	0.5 weight fraction of	1.0 weight fraction of
		bisphen_dimeth_carbo	bisphen_dimeth_carbo	bisphen_dimeth_carbo
		nate	nate	nate
Refractive index	0	1.712	1.644	1.587
Volume resistivity	Ohm- metre	4915633000000000.000	296200900000000000.000	1550173000000000000.000

Centurion Journal of Multidisciplinary Research Special issue: Nov 2020

ISSN: 2395-6216