Elastic moduli of pristine clay minerals and clay polymer hybrids

Sanam Bashir [1*], Daniel Moreno-Rodriguez[1], Peter Škorňa[1], Eva Scholtzová [1]

[1]Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36 Bratislava, Slovakia

[*]uachsnam@savba.sk

Abstract

Over the past few decades, there has been a growing interest in hybrid materials possessing exceptional properties, as they have the potential to replace traditional materials in various engineering applications. Consequently, the extensive exploration of intercalating organic molecules into layered materials like clay minerals has been a prominent area of research for an extended period [1]. Specifically, the adsorption of polymers into clay minerals has been a subject of extensive investigation, primarily due to the abundant availability and biocompatible nature of clay minerals. Furthermore, their chemical and mechanical stability, high surface area, cationic exchange capacity, and structural characteristics makes them highly suitable for a wide range of applications[2].

Only small amount of clay minerals (5 wt%) can dramatically improve the overall characteristics of the clay polymer hybrids. Due to high interfacial area, stress is transferred from polymer to clay minerals resulting in high mechanical strength of the clay polymer hybrids. Thus, the motivation for studying the intercalation of a polymer into the clay minerals is to develop a clay polymer hybrid with enhanced mechanical strength[3].

In this present work we predict and compare the interaction between montmorillonite (Na-Mt) and beidellite (Na-Bd) clay with the pentamer of nonionic polymer (poly2-methyl-2-oxazoline or PMeOx) using computational methods. DFT-D3 calculations were used to study the structural stability of two structural models (Na-Mt-PMeOx and Na-Bd-PMeOx). Further, this study investigated the elastic moduli such as bulk, shear and young's modulus of the pristine clay minerals (Na-Mt and Na-Bd,) and clay-polymer hybrids (Na-Mt-PMeOx and Na-Bd-PMeOx) for the better understanding of their mechanical properties.

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