

عنوان مقاله:

Molecular Dynamic Simulation of Polymer-Clay Nanocomposites Containing Positive ion of Adenine

محل انتشار:

سومین همایش ملی کاربردهای شیمی در فناوریهای نوین (سال: 1392)

تعداد صفحات اصل مقاله: 5

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خلاصه مقاله:

In this research, the polymer-clay nanocomposites which the positive ion of adenine located between its layers instead of sodium ion were studied by molecular dynamic methods. Energy and volume of this clay were analyzed to show the effect of central adenine on clay properties. Remarkable result which obtained is that by the volume and distance of layers is considerably depends on nature of substituent attached to Adenine. However it was shown that the volume of nanoclay is nonlinearly depend on volume of substituent. On the other hand energy and volume of system was drastically affected by temperature

کلمات کلیدی:

Polymer Clay Nanocomposites, Adenine, Molecular Dynamics

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<https://civilica.com/doc/233252>

