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Prediction on Thermal Conductivity of Energetic Polymers

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Abstract: The thermal conductivity of explosives is an important index to understand the non-shock initiation and the non-ideal detonation. On the basis of experimental thermal conductivity data of polymers, two methods for calculating thermal conductivity, which are proposed by Bicerano and Askadskii, respectively, are compared. By calculating and comparing the relative deviations, Askadskii group contribution method is verified to be efficient and thus adopted, because of its small relative deviation. Based on the analysis results of the structures, properties and thermal conduction mechanism of conjugated polymers, several energetic conjugated polymers are designed by adding energetic groups $-\text{NO}_2$, $-\text{N}_3$ and $-\text{ONO}_2$ up to the conjugated polymer structures. A coupling between phonon conduction and electron conduction in the conjugate systems of energetic conjugated polymers will lead to an increase in the thermal conductivity. Thermal conductivity calculation shows that the new designed conjugated energetic polymers exhibit the enhanced thermal conductivity, above $1.0 \text{ W} \cdot \text{mK}^{-1}$.

Key words: energetic polymers; thermal conductivity; group contribution method

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《含能材料》“观点”征稿

为了丰富学术交流形式,及时传递含能材料领域同行们的学术观点和思想,《含能材料》开设了“观点”栏目。“观点”栏目的来稿应观点鲜明、内容新颖、形式上短小精悍。欢迎含能材料各领域的专家积极来稿。来稿时请附个人简介及主要研究工作介绍。

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