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Graphene layer growth: collision of migrating 5-member rings

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Abstract

A reaction pathway is explored in which two cyclopenta groups combine on the zigzag edge of a graphene layer. The process is initiated by H addition to a five-member ring, followed by opening of that ring and the formation of a six-membered ring adjacent to the other five-membered ring. The elementary steps of the migration pathway were analyzed using density functional theory to examine the region of the potential energy surface associated with the pathway. The calculations were performed on a substrate modeled by the zigzag edge of tetracene. The computed reaction energetics indicate feasibility of this reaction pathway in the growth of zigzag edge in high temperature environments.