

Bipolaron formation and desorption following Auger decay in polyacetylene. Liegener, C. M.; Foerner, W.; Ladik, J

Abstract

The Su-Schrieffer-Heeger model was applied to a trans-polyacetylene chain with 2 holes at the top of the valence band. In the kink-free chain the formation of a kink-antikink pair is obsd. This is deformed to a polaron pair due to end effects and the lack of dissipation in the model. For an end-kink configuration, desorption may occur. The influence of a substitutional NH impurity on these phenomena is discussed.