CIS-DEFECTS IN TRANS-POLYENES

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All trans-polyenes have received tremendous experimental and theoretical attention because of their importance to vision and photosynthesis as well as conductive and semiconductive electronic applications. Numerous examples exist of cis-linkages contained in an otherwise all trans-polyene unit, such as the cis-trans isomerization associated with the vision process or the cis-polyacetylene formed initially in the Shirakawa synthesis of trans-polyacetylene. Though such cis-structures can have significant impact on optical, electronic, and nonlinear optical properties, such defects have received only scant attention. In this work, we report the results of ab initio calculations on the structure and properties of cis-defects embedded within all-trans-polyene units.