Fatigue and Fatigue Resistance in S1 Excited State Diarylethenes in Electric fields

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Abstract

The effect of a directional electric-field on the bonding of the undoped and sulphur doped diarylethene (DTE) switch molecule is investigated using next generation QTAIM (NG-QTAIM). We introduce chemical bonding concepts in the form of the least and most preferred directions of charge density accumulation relative to the associated bond-path, namely the precessions K and K' that are demonstrated to be much more responsive to the electric-field than the Laplacian [?]2ρ(rb). A concept of bond fatigue is presented in terms of the tendency for a bond-path to rupture that provides directional versions of familiar bonding QTAIM concepts. Examples are included where the applied directional electric-field reduces the tendency towards bond-path rupture and also the converse. A brief discussion is undertaken of applications of the precessions K and K' including switches, ring opening reactions and molecular rotary motors in the presence of fields that cause a redistribution of ρ(r).

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