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Title: Conjugated polyacetylenes in a high-intensity circularly polarized laser

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Abstract:

In last decades, light matter interaction pushed to laser induced atomic and molecular electron dynamics. Solving Schr Ö dinger equation with laser purtubed hamiltonian by using Hartree-Fock theory brings a way to observe evoultion of molecular orbitals and their energies with time. Here, we have performed a computation where laser has been induced on polyacetylens with fixed nuclear states to observe effects to π electron delocalization. Molecular electron density (MED) which is scalar field and physically observable quantity is useful to gain knoweldge of chemical anologies from topological point of view. The topographical analysis brings out changes in number and nature of critical points corresponding to reorientation of electron cloud. Bond saddle which gives insightment to hypothetical nature of chemical bond and its bond ellipticity to measure anisotropy and π character were extensively studied and analysed with propogation. In the presence of laser, bond critical point between C and H approches towards H, providing charge redistribution, decrease in size of basin and AIM atomic charge and so increase in electropositive charactor for H attractor, bond polarity of C-H bond and overall acidity of molecule. Slight shift to higher intensity regime affects MED bifurcating acetylenic bcp, forming more regions, basins and active reaction sites.

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