Original Paper | Published: 31 March 2020

Solitonic-like excitations in cations of linear conjugated systems

Kateryna O. Maiko, Igor M. Dmitruk, Nataliya V. Obernikhina & Aleksey D. Kachkovsky

Monatshefte für Chemie - Chemical Monthly **151**, 559–566 (2020) | Cite this article

Abstract

A quantum-chemical study of the atomic charges and bond orders in the cations of the linear conjugated systems was performed. It is shown that total charge in the collective system of the π-electrons generates the soliton-like wave of the alternated partial charges along the conjugated chain not only in ground state but also in the excited state. The excitation is accompanied by the change of the soliton phase and the wave dimension. Additionally, it is established that the electron density redistribution at the atoms and bonds also forms the soliton-like wave. In paper, the dependence of the solitonic wave shape on the dimension and section of the polymethine is studied; established regularities in the charge distribution in excited state could be used for the molecular design of organic semiconducting materials.

Graphic abstract